Synthesis of Chiral α-Amino Tertiary Boronates via the Catalytic Enantioselective Nucleophilic Borylation of Dialkyl Ketimines

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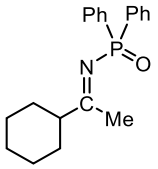
1. General and Materials

All reactions were performed in oven-dried glassware using conventional Schlenk techniques under a static pressure of nitrogen or argon. Materials were obtained from commercial suppliers and used as received unless otherwise noted. Dry solvents for the reactions were purchased from commercial suppliers, degassed via three freeze-pump-thaw cycles, and further dried over molecular sieves (MS4A) prior to use. 1,3-Dicyclohexylimidazolium chloride (ICy·HCl, >98.0%) and K(O-*t*-Bu) (>97.0%) purchased from Tokyo Chemical Industry Co. The chiral *N*-heterocyclic carbene (NHC) ligand precursors (*R*,*S*)-**L1,** (*R*,*S*)-**L2,** (*R*,*S*)-**L3** were purchased from Strem Chemicals, Inc. [(*S*,*S*)-**L4**-(*S*,*S*)-**L7**[1], (*S*,*S*)-**L8**[2], (*S*,*S*)-**L9**[2] and (*R*,*R*)-**L10**[3]] were synthesized according to the literature. (*R*)-DTBM-SEGPHOS [(*R*)-**L11**] was purchased from Tokyo Chemical Industry Co. (*R*,*R*)-Quinox P* [(*R*,*R*)-**L12**] was obtained from Nippon Chemical Industrial Co. Silica Gel 60 N (40–100 μm, spherical, neutral) purchased from Kanto Chemical Co. was used as received. NMR spectra were recorded on JEOL JNM-ECX400P, ECS-400 (^{1}H: 392 or 396 MHz, ^{13}C: 99 or 100 MHz), and JNM-ECA600 (^{13}C: 151 MHz). Tetramethylsilane (δ = 0.00 ppm for ^{1}H NMR) and $CDCl_3$ (δ = 77.0 ppm for ^{13}C NMR) were employed as external standards. $BF_3 \cdot Et_2O$ was used as an external standard for ^{11}B NMR analysis. D_3PO_4 in D_2O was used as an external standard for ^{31}P NMR analysis. Multiplicity was reported as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, m = multiplet. 1,1,2,2-Tetrachloroethane was used as an internal standard for determining NMR yield. NMR yield was determined by quantitative ^{1}H-NMR analysis of the crude reaction mixture. GLC analyses were conducted with a Shimadzu GC-2014 or GC-2025 equipped with ULBON HR-1 glass capillary column (Shinwa Chemical Industries) and an FID detector. Recycle preparative gel chromatography (GPC) was conducted with JAILC-9101 using $CHCl_3$ as an eluent. FTIR spectra were recorded on a JASCO FT IR 4700 spectrometer. Single crystal X-ray structural analyses were carried out on an XtaLAB PRO MM007 diffractometer using graphite monochromated Cu- K_α radiation. The structure was solved by direct methods and expanded using Fourier techniques. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the Olex2 crystallographic software package except for refinement, which was performed using SHELXL-2013. High-resolution mass spectra were recorded at the Global Facility Center for Instrumental Analysis, Hokkaido University.

2. Substrate Synthesis

List of the substrate used in this study.



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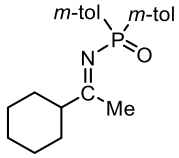

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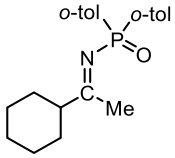

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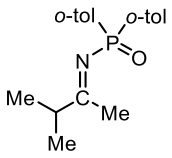

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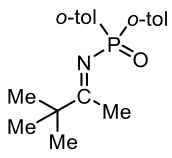

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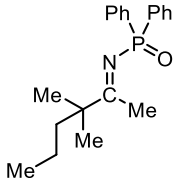

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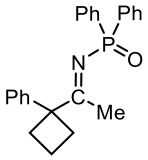

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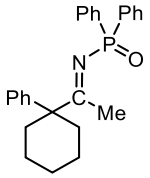

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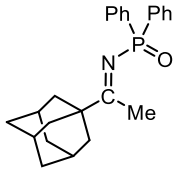

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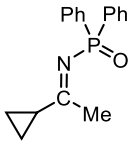

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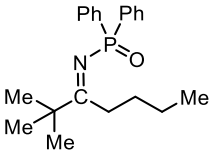

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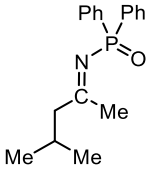

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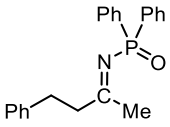

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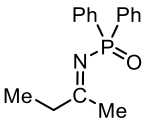
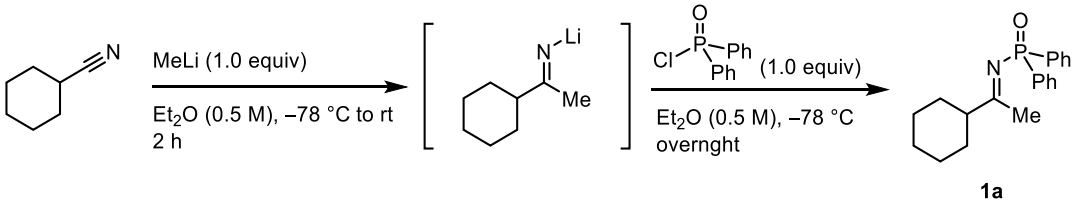


1n

The spectroscopic data of **1a** and **1e** were consistent with literature values.[4,5] The *E*/*Z* configurations of other substrates were deduced relative to these compounds.

Procedure A.

(*E*)-*N*-(1-Cyclohexylethylidene)-*P*,*P*-diphenylphosphinic amide (1a).



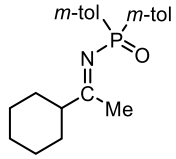
1a

MeLi (Et_2O 1.1 M) (9.1 mL, 10 mmol, 1.0 equiv) was added dropwise to a suspension of cyclohexanecarbonitrile (1.2 mL, 10 mmol, 1.0 equiv) in Et_2O (20 mL) at −78 °C under nitrogen atmosphere. The reaction mixture was allowed to warm to room temperature and stirred for 2 h. Then, the reaction mixture was cooled down to −78 °C, and diphenyl phosphinic chloride (1.91 mL, 10 mmol, 1.0 equiv) was added dropwise to the mixture. The reaction mixture was kept at −78 °C and stirred

overnight. The mixture was directly filtered through a short silica-gel column with EtOAc as an eluent, and then the resultant solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with EtOAc/Hex eluent (100:0 to 30:70). Further purification was conducted by GPC to afford the corresponding ketimine **1a** (280.5 mg, 0.86 mmol, 9% yield) as a white solid. The spectroscopic data were matched in those reported.[4]

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.17–1.46 (m, 5H), 1.71–1.95 (m, 5H), 2.35–2.43 (m, 1H), 2.47 (d, *J* = 1.6 Hz, 3H), 7.39–7.47 (m, 6H), 7.89–7.94 (m, 4H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{20}H_{24}NOP$, 325.1596; found, 325.1598.

(*E*)-*N*-(1-Cyclohexylethylidene)-*P*,*P*-di-*m*-tolylphosphinic amide (1b).

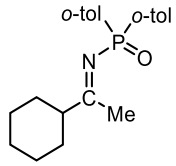


1b

1b was prepared from the corresponding nitrile according to procedure A. The product **1b** was obtained in 26% yield (373.7 mg, 1.1 mmol, yellow oil) from the corresponding nitrile (4.0 mmol).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.19–1.49 (m, 5H), 1.70–1.94 (m, 5H), 2.36 (s, 6H), 2.38–2.42 (m, 1H), 2.45 (d, *J* = 2.4 Hz, 3H), 7.24–1.34 (m, 4H), 767–7.76 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 21.5 (*C*H_3), 25.2 (d, *J* = 13.4 Hz, *C*H_3), 25.99 (*C*H_2), 26.04 (*C*H_2), 30.2 (*C*H_2), 52.1 (d, *J* = 20.1 Hz, *C*H), 128.2 (d, *J* = 13.4 Hz, *C*H), 128.7 (d, *J* = 8.6 Hz, *C*H), 132.0 (d, *J* = 5.8 Hz, *C*H), 132.1 (*C*H), 134.9 (d, *J* = 130.3 Hz, *C*), 138.1 (d, *J* = 13.4 Hz, *C*), 195.4 (d, *J* = 11.5 Hz, *C*). ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 18.4. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{28}NOP$, 353.1909; found, 353.1908. IR (neat, cm^{-1}): 1187 (P=O), 1652 (C=N).

(*E*)-*N*-(1-Cyclohexylethylidene)-*P*,*P*-di-*o*-tolylphosphinic amide (1c).



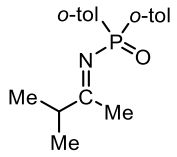
1c

1c was prepared from the corresponding nitrile according to procedure A. The product **1c** was obtained in 4% yield (187.4 mg, 0.50 mmol, white solid) from the corresponding nitrile (13.6 mmol).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.22–1.39 (m, 5H), 1.70–1.94 (m, 5H), 2.30 (s, 6H), 2.34–2.39 (m, 1H), 2.41 (d, *J* = 1.8 Hz, 3H), 7.14–7.17 (m, 2H), 7.28–7.30 (m, 2H), 7.35–7.41 (m, 2H), 8.08 (ddd, *J*

= 1.0, 7.8, 15.7 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 21.7 (d, J = 2.9 Hz, CH_3), 25.3 (d, J = 14.2 Hz, CH_3), 26.1 (CH_2), 30.3 (CH_2), 52.6 (d, J = 20.8 Hz, *C*H), 125.4 (d, J = 12.3 Hz, *C*H), 131.4 (d, J = 12.3 Hz, *C*H), 131.6 (d, J = 1.9 Hz, *C*H), 132.6 (d, J = 123.8 Hz, *C*), 133.4 (d, J = 9.5 Hz, *C*H), 141.5 (d, J = 10.3 Hz, *C*), 196.3 (d, J = 11.3 Hz, *C*). ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 20.3. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{28}NOP$, 353.1909; found, 353.1903. mp 95–100 °C. IR (neat, cm^{-1}): 1186 (P=O), 1652 (C=N).

(*E*)-*N*-(3-Methylbutan-2-ylidene)-*P*,*P*-di-*o*-tolylphosphinic amide (1d).

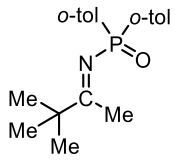


1d

1d was prepared from the corresponding nitrile according to procedure A. The product **1d** was obtained in 9% yield (146.2 mg, 0.45 mmol, white solid) from the corresponding nitrile (5.0 mmol).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.17 (d, J = 6.7 Hz, 6H), 2.30 (s, 6H), 2.42 (d, J = 2.0 Hz, 3H), 2.72 (h, J = 6.9 Hz, 1H), 7.14–7.17 (m, 2H), 7.26–7.30 (m, 2H), 7.35–7.39 (m, 2H), 8.09 (ddd, J = 1.4, 5.9, 13.7 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 19.9 (CH_3), 21.6 (d, J = 3.8 Hz, CH_3), 24.9 (d, J = 14.2 Hz, CH_3), 42.4 (d, J = 20.8 Hz, *C*H), 125.4 (d, J = 11.3 Hz, *C*H), 131.4 (d, J = 12.3 Hz, *C*H), 131.6 (d, J = 1.9 Hz, *C*H), 132.5 (d, J = 124.6 Hz, *C*), 133.4 (d, J = 8.5 Hz, *C*H), 141.5 (d, J = 10.4 Hz, *C*), 196.9 (d, J = 11.4 Hz, *C*). ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 20.4. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{19}H_{24}NOP$, 313.1596; found, 313.1593. mp 108–111 °C. IR (neat, cm^{-1}): 1188 (P=O), 1658 (C=N).

(*E*)-*N*-(3,3-Dimethylbutan-2-ylidene)-*P*,*P*-di-*o*-tolylphosphinic amide (1e).

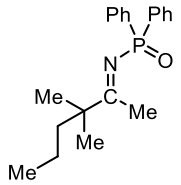


1e

1e was prepared from the corresponding nitrile according to procedure A. The product **1e** was obtained in 32% yield (414.6 mg, 1.27 mmol, white solid) from the corresponding nitrile (4.0 mmol). The spectroscopic data were matched in those reported.[5]

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.22 (s, 9H), 2.28 (s, 6H), 2.43 (d, J = 1.8 Hz, 3H), 7.13–7.17 (m, 2H), 7.26–7.30 (m, 2H), 7.35–7.39 (m, 2H), 8.09 (dd, J = 1.8, 7.6 Hz, 2H), 8.12 (dd, J = 1.4, 7.6 Hz, 2H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{20}H_{26}NOP$, 325.1752; found, 327.1746.

(*E*)-*N*-(3,3-Dimethylhexan-2-ylidene)-*P*,*P*-diphenylphosphinic amide (1f).

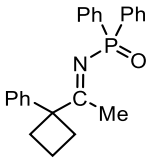


1f

1f was prepared from the corresponding nitrile according to procedure A. The product **1f** was obtained in 44% yield (579.3 mg, 1.77 mmol, white solid) from the corresponding nitrile (4.0 mmol).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.84 (t, J = 7.4 Hz, 3H), 1.09–1.18 (m, 2H), 1.20 (s, 6H), 1.54–1.58 (m, 2H), 2.46 (d, J = 1.6 Hz, 3H), 7.38–7.47 (m, 6H), 7.89–7.94 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.8 (*C*H_3), 18.1 (*C*H_2), 22.1 (d, J = 13.4 Hz, *C*H_3), 25.9 (*C*H_3), 43.5 (*C*H_2), 47.3 (d, J = 20.1 Hz, *C*), 128.4 (d, J = 12.5 Hz, *C*H), 131.3 (d, J = 2.9 Hz, *C*H), 131.6 (d, J = 9.6 Hz, *C*H), 135.1 (d, J = 131.2 Hz, *C*), 197.7 (d, J = 12.4 Hz, *C*). ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 17.3. HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{20}H_{27}NOP$, 328.1825; found, 328.1823. mp 56–61 °C. IR (neat, cm^{-1}): 1203 (P=O), 1650 (C=N).

(*E*)-*P*,*P*-Diphenyl-*N*-[1-(1-phenylcyclobutyl)ethylidene]phosphinic amide (1g).

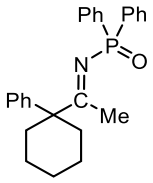


1g

1g was prepared from the corresponding nitrile according to procedure A. The product **1g** was obtained in 28% yield (416.6 mg, 1.12 mmol, white solid) from the corresponding nitrile (4.0 mmol).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.89 (quint, J = 13.2 Hz, 2H), 2.23 (d, J = 2.0 Hz, 3H), 2.50–2.57 (m, 2H), 2.83–2.90 (m, 2H), 7.17–7.31 (m, 5H), 7.42–7.50 (m, 6H), 7.96 (ddd, J = 1.5, 5.9, 9.8 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 15.9 (*C*H_2), 21.9 (d, J = 12.4 Hz, *C*H_3), 31.9 (*C*H_2), 59.1 (d, J = 22.1 Hz, *C*), 126.4 (*C*H), 126.8 (*C*H), 128.4 (*C*H), 128.6 (d, J = 8.6 Hz, *C*H), 131.5 (d, J = 2.8 Hz, *C*H), 131.6 (d, J = 8.6 Hz, *C*H), 134.9 (d, J = 130.3 Hz, *C*), 144.0 (*C*), 193.3 (d, J = 11.5 Hz, *C*). ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 18.5. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{24}H_{24}NOPNa$, 396.1488; found, 396.1486. mp 88–96 °C. IR (neat, cm^{-1}): 1204 (P=O), 1655 (C=N).

(*E*)-*P*,*P*-Diphenyl-*N*-[1-(1-phenylcyclohexyl)ethylidene]phosphinic amide (1h).

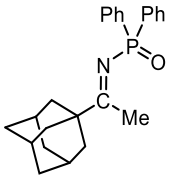


1h

1h was prepared from the corresponding nitrile according to procedure A. The product **1h** was obtained in 35% yield (567.9 mg, 1.41 mmol, white solid) from the corresponding nitrile (4.0 mmol).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 1.37–1.58 (m, 6H), 2.01–2.08 (m, 2H), 2.24 (d, *J* = 2.4 Hz, 3H), 2.31–2.35 (m, 2H), 7.16–7.30 (m, 5H), 7.42–7.52 (m, 6H), 7.92–7.98 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 22.9 (d, *J* = 13.4 Hz, *C*H_3), 23.0 (*C*H_2), 26.1 (*C*H_2), 34.4 (*C*H_2), 54.9 (d, *J* = 20.1 Hz, *C*), 126.8 (*C*H), 126.9 (*C*H), 128.5 (d, *J* = 12.4 Hz, *C*H), 128.7 (*C*H), 131.5 (d, *J* = 2.9 Hz, *C*H), 131.7 (d, *J* = 9.6 Hz, *C*H), 134.6 (d, *J* = 130.3 Hz, *C*), 143.5 (*C*), 194.5 (d, *J* = 12.5 Hz, *C*). ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 18.4. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{26}H_{28}NOP$, 401.1909; found, 401.1897. mp 103–106 °C. IR (neat, cm^{-1}): 1198, 1211 (P=O), 1651 (C=N).

***N*-{(*E*)-1-[(3r,5r,7r)-Adamantan-1-yl]ethylidene}-*P*,*P*-diphenylphosphinic amide (1i).**

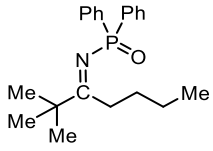


1i

1i was prepared from the corresponding nitrile according to procedure A. The product **1i** was obtained in 10% yield (157.0 mg, 0.42 mmol, white solid) from the corresponding nitrile (4.0 mmol).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.75 (q, *J* = 13.2 Hz, 6H), 1.88 (d, *J* = 2.7 Hz, 6H), 2.09 (s, 3H), 2.45 (d, *J* = 2.0 Hz, 3H), 7.38–7.47 (m, 6H), 7.90–7.96 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 21.2 (d, *J* = 13.3 Hz, *C*H_3), 28.3 (*C*H), 36.7 (*C*H_2), 39.5 (*C*H_2), 45.9 (d, *J* = 19.8 Hz, *C*), 128.4 (d, *J* = 12.3 Hz, *C*H), 131.2 (d, *J* = 2.8 Hz, *C*H_3), 131.6 (d, *J* = 9.4 Hz, *C*H_3), 135.3 (d, *J* = 130.3 Hz, *C*), 197.9 (d, *J* = 11.3 Hz, *C*). ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 17.6. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{24}H_{28}NOP$, 377.1909; found, 377.1908. mp 170–172 °C. IR (neat, cm^{-1}): 1202 (P=O), 1651 (C=N).

(*E*)-*N*-(2,2-Dimethylheptan-3-ylidene)-*P*,*P*-diphenylphosphinic amide (1k).

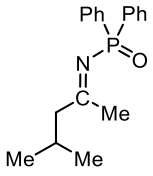


1k

1k was prepared from the corresponding nitrile according to the procedure A. The product **1k** was obtained in 66% yield (905.7 mg, 2.65 mmol, white solid) from the corresponding nitrile (4.0 mmol).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.86 (t, J = 7.1 Hz, 3H), 1.26 (s, 9H), 1.38 (quint, J = 7.3 Hz, 2H), 1.45–1.53 (m, 2H), 2.80–2.84 (m, 2H), 7.37–7.46 (m, 6H), 7.91–7.96 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 13.7 (*C*H_3), 23.4 (*C*H_2), 28.0 (*C*H_3), 31.3 (*C*H_2), 35.3 (d, J = 11.5 Hz, *C*H_2), 44.2 (d, J = 21.1 Hz, *C*), 128.4 (d, J = 12.4 Hz, *C*H), 131.2 (d, J = 2.9 Hz, *C*H), 131.6 (d, J = 8.6 Hz, *C*H), 135.6 (d, J = 132.2 Hz, *C*), 200.8 (d, J = 12.4 Hz, *C*). ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 15.6. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{21}H_{28}NOP$, 341.1909; found, 341.1912. mp 67–70 °C. IR (neat, cm^{-1}): 1199 (P=O), 1650 (C=N).

(*E*)-*N*-(4-Methylpentan-2-ylidene)-*P*,*P*-diphenylphosphinic amide (1l).



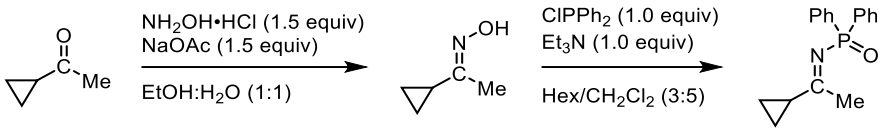
1l

1l was prepared from the corresponding nitrile according to procedure A. The product **1l** was obtained in 25% yield (302.0 mg, 1.0 mmol, white solid) from the corresponding nitrile (4.0 mmol).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.94 (d, J = 7.1 Hz, 6H), 2.17–2.31 (m, 1H), 2.43–2.45 (m, 5H), 7.39–7.48 (m, 6H), 7.89–7.95 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 22.7 (*C*H_3), 26.3 (*C*H), 27.6 (d, J = 15.4 Hz, *C*H_3), 53.2 (d, J = 28.1 Hz, *C*H_2), 128.4 (d, J = 12.4 Hz, *C*H), 131.4 (d, J = 2.0 Hz, *C*H), 131.7 (d, J = 9.5 Hz, *C*H), 134.9 (d, J = 130.3 Hz, *C*), 191.9 (d, J = 10.6 Hz, *C*). ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$, δ): 22.3. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{18}H_{22}NOP$, 299.1439; found, 299.1431. mp 166–168 °C. IR (neat, cm^{-1}): 1180 (P=O), 1555 (C=N).

Procedure B.

(*E*)-*N*-(1-Cyclopropylethylidene)-*P*,*P*-diphenylphosphinic amide (1j).

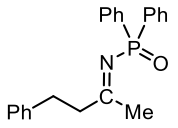


1j

1-Cyclopropylethan-1-one (841.0 mg, 10 mmol, 1.0 equiv) was added to a stirred solution of $NH_2OH{\cdot}HCl$ (1.04 g, 15 mmol, 1.5 equiv) and NaOAc (1.23 g, 15 mmol, 1.5 equiv) in EtOH/H_2O (1/1, 10 mL), and then heated to reflux. When the reaction was completed, the mixture was cooled down to ambient temperature. The reaction mixture was then diluted with Na_2CO_3 saturated aqueous solution and extracted with CH_2Cl_2 three times, and dried over $MgSO_4$. After filtration, the obtained oxime was dried under vacuum overnight and used directly for the next process without purification. A solution of chlorodiphenylphosphine (1.04 mL, 6.0 mmol, 1.0 equiv) in CH_2Cl_2 (6 mL) was added to a stirred solution of the oxime (597.5 mg, 6.0 mmol, 1.0 equiv) and triethylamine (836 μL, 6.0 mmol, 1.0 equiv) in petroleum ether/CH_2Cl_2 (1:1, 9 mL) over 1 h at −45 °C. After the addition was finished, the cooling bath was removed, and the reaction temperature was gradually increased. The mixture was then allowed to stir overnight at ambient temperature. The mixture was directly filtered through a short silica-gel column with EtOAc as an eluent; then the resultant solution was concentrated under reduced pressure. The residue was purified by GPC to afford the corresponding ketimine **1j** (130.2 mg, 0.46 mmol, 8% yield) as a white solid.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.99–1.04 (m, 2H), 1.15–1.18 (m, 2H), 1.93–2.00 (m, 1H), 2.54 (d, J = 2.0 Hz, 3H), 7.38–7.45 (m, 6H), 7.83–7.89 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 12.3 (CH_2), 22.7 (d, J = 24.6 Hz, *C*H), 26.9 (d, J = 13.3 Hz, CH_3), 128.3 (d, J = 12.3 Hz, *C*H), 131.2 (d, J = 1.9 Hz, *C*H), 131.4 (d, J = 8.5 Hz, *C*H), 135.1 (d, J = 131.3 Hz, *C*), 194.1 (d, J = 7.5 Hz, *C*). ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$, δ): 18.4. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{17}H_{18}NOP$, 283.1126; found, 283.1120. mp 118–122 °C. IR (neat, cm^{-1}): 1183, 1194 (P=O), 1652 (C=N).

(*E*)-*P*,*P*-Diphenyl-*N*-(4-phenylbutan-2-ylidene)phosphinic amide (1m).

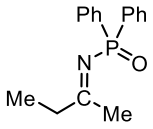


1m

1m was prepared from the corresponding ketone according to procedure B. The product **1m** was obtained in 7% yield (127.7 mg, 0.37 mmol, white solid) from the corresponding oxime (5.0 mmol). The spectroscopic data were matched in those reported[6].

^{1}H NMR (392 MHz, $CDCl_3$, δ): 2.47 (d, *J* = 1.6 Hz, 3H), 2.90 (t, *J* = 7.3 Hz, 2H), 3.04 (t, *J* = 7.4 Hz, 2H), 7.19–7.28 (m, 5H), 7.38–7.50 (m, 6H), 7.83–7.88 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 27.3 (d, *J* = 14.2 Hz, *C*H_3), 31.7 (*C*H_2), 45.1 (d, *J* = 20.7 Hz, *C*H_2), 126.2 (*C*H), 128.31 (*C*H), 128.33 (*C*H), 128.5 (d, *J* = 11.4 Hz, *C*H), 131.4 (d, *J* = 2.8 Hz, *C*H), 131.6 (d, *J* = 9.4 Hz, *C*H), 134.6 (d, *J* = 130.3 Hz, *C*), 140.1 (*C*), 190.8 (d, *J* = 10.3 Hz, *C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{22}NOP$, 347.1439; found, 347.1430.

(*E*)-*N*-(Butan-2-ylidene)-*P*,*P*-diphenylphosphinic amide (1n).

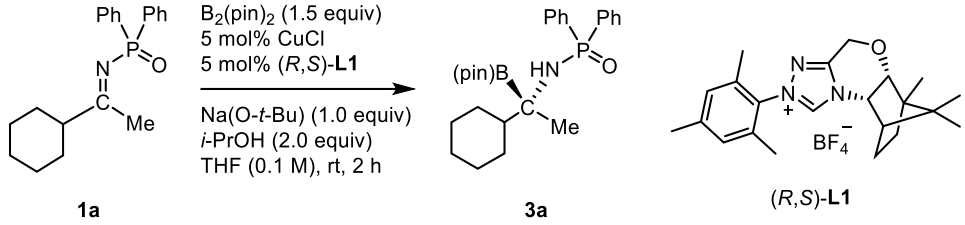


1n

1n was prepared from the corresponding ketone according to procedure B. The product **1n** was obtained in 5% yield (102.8 mg, 0.38 mmol, white solid) from the corresponding oxime (8.0 mmol).

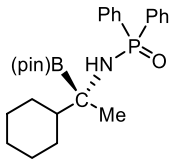
^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.20 (t, *J* = 7.3 Hz, 3H), 2.46 (d, *J* = 2.0 Hz, 3H), 2.58 (q, *J* = 7.3 Hz, 2H), 7.39–7.48 (m, 6H), 7.90–7.96 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 10.2 (*C*H_3), 26.9 (d, *J* = 14.2 Hz, *C*H_3), 37.4 (d, *J* = 20.8 Hz, *C*H_2), 128.5 (d, *J* = 12.3 Hz, *C*H), 131.4 (d, *J* = 2.9 Hz, *C*H), 131.7 (d, *J* = 9.5 Hz, *C*H), 135.0 (d, *J* = 131.3 Hz, *C*), 192.8 (d, *J* = 10.4 Hz, *C*). ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$, δ): 22.4. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{16}H_{18}NOP$, 271.1126; found, 271.1121. mp 161–168 °C. IR (neat, cm^{-1}): 1179 (P=O), 1557 (C=N).

3. General Experimental Procedures for Borylation of Ketimines



CuCl (1.0 mg, 0.01 mmol, 5 mol %), (*R*,*S*)-**L1** (4.4 mg, 0.01 mmol, 5 mol %), and bis(pinacolato)diboron (76.2 mg, 0.30 mmol, 1.5 equiv) were placed in a vial with a screw cap containing a Teflon®-coated rubber septum under air. The vial was put in a glove box, and then Na(O-*t*-Bu) (19.2 mg, 0.20 mmol, 1.0 equiv) was also added to the vial in the glove box under an argon atmosphere. After the reaction, the vial was removed from the glove box, THF (0.6 mL) was added to the vial via a syringe. The resulting mixture was stirred for 10 min at room temperature, then a THF solution (1.4 mL) of ketimine **1a** (65.0 mg, 0.20 mmol, 1.0 equiv) was added dropwise to the vial. *i*-PrOH (31 μL, 0.40 mmol, 2.0 equiv) was added to the reaction mixture. After the resulting mixture was stirred at room temperature for 2 h, the reaction mixture was analyzed by GC to check the completeness of the reaction. The mixture was directly filtered through a short silica-gel column with EtOAc as an eluent; then the resultant solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane/EtOAc eluent (100:0 to 40:60). After silica-gel column purification, the mixture was further purified by extraction with CH_2Cl_2 and H_2O three times to remove pinacol. The CH_2Cl_2 solution was dried over $MgSO_4$. After filtration, the corresponding product **3a** was obtained in 86% yield (78.0 mg, 0.17 mmol) as a colorless oil. The racemic sample was prepared using ICy·HCl for the ligand instead of (*R*,*S*)-**L1**.

(*R*)-*N*-[1-Cyclohexyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl]-*P*,*P*-diphenylphosphinic amide [(*R*)-3a].

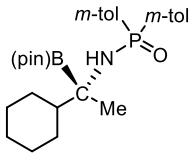


(*R*)-**3a**

The reaction was conducted with 65.1 mg (0.20 mmol) of **1a**. The product (*R*)-**3a** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→40:60) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3a** was obtained in 86% yield (78.0 mg, 0.17 mmol, colorless oil) with 89% ee.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 1.01–1.26 (m, 5H), 1.17 (s, 3H), 1.29 (s, 6H) 1.30 (s, 6H), 1.44–1.50 (m, 1H), 1.64–1.89 (m, 5H), 3.04 (d, J = 7.9 Hz, 1H), 7.38–7.48 (m, 6H), 7.80–7.88 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 19.6 (d, J = 3.9 Hz, CH_3), 25.0 (CH_3), 25.1 (CH_3), 26.76 (CH_2), 26.81 (d, J = 1.9 Hz, CH_2), 28.5 (d, J = 42.6 Hz, CH_2), 47.5 (d, J = 4.4 Hz, *C*H), 49.5 (br, B-*C*), 84.2 (*C*), 128.2 (*C*H), 128.4 (*C*H), 131.3 (*C*H), 131.8 (d, J = 9.5 Hz, *C*H), 132.0 (d, J = 9.4 Hz, *C*H), 135.3 (d, J = 6.6 Hz, *C*), 136.6 (d, J = 5.7 Hz, *C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 33.1. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 21.9. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{26}H_{37}{}^{11}BNO_3PNa$, 476.2501; found, 476.2496. $[\alpha]_D^{21.0}$ –6.59 (*c* 1.10 in $CHCl_3$, 89% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 11.97 min., *R* isomer: t_R = 15.01 min. IR (neat, cm^{-1}): 1200 (P=O).

(*R*)-*N*-[1-Cyclohexyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl]-*P*,*P*-di-*m*-tolylphosphinic amide [(*R*)-3b].



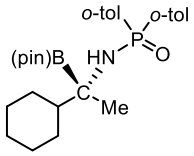
(*R*)-**3b**

The reaction was conducted with 71 mg (0.20 mmol) of **1b** for 2 h. The product (*R*)-**3b** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→40:60) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3b** was obtained in 74% yield (70.6 mg, 0.15 mmol, colorless oil) with 90% ee.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.01–1.24 (m, 5H), 1.17 (s, 3H), 1.29 (s, 6H), 1.31 (s, 6H), 1.43–1.50 (m, 1H), 1.56–1.94 (m, 5H), 2.36 (s, 6H), 3.02 (d, J = 7.8 Hz, 1H), 7.26–7.34 (m, 4H), 7.57–7.62 (m, 2H), 7.70 (dd, J = 4.5, 12.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 19.5 (d, J = 3.8 Hz, CH_3),

21.5 (*C*H$_3$), 25.0 (*C*H$_3$), 25.1 (*C*H$_3$), 26.76 (*C*H$_2$), 26.82 (d, *J* = 2.9 Hz, *C*H$_2$), 28.4 (d, *J* = 47.9 Hz, *C*H$_2$), 47.5 (d, *J* = 3.9 Hz, *C*H), 49.5 (br, B-*C*), 84.2 (*C*), 128.1 (d, *J* = 3.9 Hz, *C*H), 128.2 (d, *J* = 3.8 Hz, *C*H), 128.8 (d, *J* = 10.6 Hz, *C*H), 128.9 (d, *J* = 10.5 Hz, *C*H), 131.98 (d, *J* = 2.9 Hz, *C*H), 132.01 (d, *J* = 2.8 Hz, *C*H), 135.2 (d, *J* = 13.4 Hz, *C*), 136.5 (d, *J* = 11.5 Hz, *C*), 138.0 (d, *J* = 12.4 Hz, *C*). ^{11}B{^{1}H} NMR (127 MHz, CDCl$_3$, δ): 33.5. ^{31}P{^{1}H} NMR (159 MHz, CDCl$_3$, δ): 22.3. HRMS-ESI (*m*/*z*): [M+Na]$^+$ calcd for $C_{28}H_{41}{}^{11}BNO_3PNa$, 504.2814; found, 504.2814. $[\alpha]_D^{25.1}$ +1.24 (*c* 1.45 in CHCl$_3$, 90% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 10.21 min., *R* isomer: t_R = 11.23 min. IR (neat, cm^{-1}): 1193 (P=O).

(*R*)-*N*-[1-Cyclohexyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl]-*P*,*P*-di-*o*-tolylphosphinic amide [(*R*)-3c].

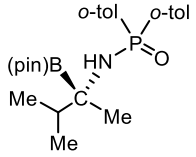


(*R*)-**3c**

The reaction was conducted with 69.2 mg (0.20 mmol) of **1c** for 3 h. The product (*R*)-**3a** was purified by flash column chromatography (SiO$_2$, CH$_2$Cl$_2$/Et$_2$O, 100:0→80:20) and obtained in 92% yield (86.3 mg, 0.18 mmol, colorless oil) with 95% ee.

^{1}H NMR (396 MHz, CDCl$_3$, δ): 1.03–1.24 (m, 5H), 1.26 (s, 6H), 1.28 (s, 6H), 1.34 (s, 3H), 1.60–1.91 (m, 6H), 2.44 (s, 3H), 2.57 (s, 3H), 2.80 (d, *J* = 11.5 Hz, 1H), 7.14–7.24 (m, 4H), 7.35 (q, *J* = 7.8 Hz, 2H), 7.53 (ddd, *J* = 1.0, 7.9, 11.9 Hz, 1H), 7.89 (ddd, *J* = 1.2, 7.9, 15.8 Hz, 1H). ^{13}C NMR (99 MHz, CDCl$_3$, δ): 20.0 (d, *J* = 2.9 Hz, *C*H$_3$), 21.7 (d, *J* = 3.8 Hz, *C*H$_3$), 22.0 (d, *J* = 3.8 Hz, *C*H$_3$), 25.0 (*C*H$_3$), 25.1 (*C*H$_3$), 26.76 (*C*H$_2$), 26.84 (*C*H$_2$), 28.7 (d, *J* = 64.3 Hz, *C*H$_2$), 48.1 (d, *J* = 3.8 Hz, *C*H), 49.6 (br, B-*C*), 84.1 (*C*), 124.9 (d, *J* = 12.3 Hz, *C*H), 125.1 (d, *J* = 12.3 Hz, *C*H), 131.19 (d, *J* = 2.8 Hz, *C*H), 131.23 (d, *J* = 2.9 Hz, *C*H), 131.5 (d, *J* = 12.3 Hz, *C*H), 131.7 (d, *J* = 11.3 Hz, *C*H), 132.9 (d, *J* = 11.3 Hz, *C*H), 133.61 (d, *J* = 29.2 Hz, *C*), 133.67 (d, *J* = 10.4 Hz, *C*H), 134.8 (d, *J* = 32.2 Hz, *C*), 142.0 (d, *J* = 9.4 Hz, *C*), 142.1 (d, *J* = 10.4 Hz, *C*). ^{11}B{^{1}H} NMR (127 MHz, CDCl$_3$, δ): 33.6. ^{31}P{^{1}H} NMR (159 MHz, CDCl$_3$, δ): 27.2. HRMS-ESI (*m*/*z*): [M+Na]$^+$ calcd for $C_{28}H_{41}{}^{11}BNO_3PNa$, 504.2814; found, 504.2814. $[\alpha]_D^{23.6}$ –26.5 (*c* 0.26 in CHCl$_3$, 95% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 8.77 min., *R* isomer: t_R = 9.57 min. IR (neat, cm^{-1}): 1192 (P=O).

(*R*)-*N*-[3-Methyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butan-2-yl]-*P*,*P*-di-*o*-tolylphosphinic amide [(*R*)-3d].

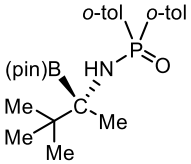


(*R*)-**3d**

The reaction was conducted with 63.7 mg (0.20 mmol) of **1d** for 2 h. The product (*R*)-**3d** was purified by flash column chromatography (SiO_2, CH_2Cl_2/Et_2O, 100:0→80:20) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3d** was obtained in 91% yield (81.8 mg, 0.19 mmol, colorless oil) with 97% ee.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 0.98 (d, *J* = 6.7 Hz, 3H), 1.01 (d, *J* = 6.7 Hz, 3H), 1.25 (s, 6H), 1.27 (s, 6H), 1.32 (s, 3H), 1.93–2.02 (m, 1H), 2.43 (s, 3H), 2.56 (s, 3H), 2.75 (d, *J* = 10.7 Hz, 1H), 7.14–7.24 (m, 4H), 7.30–7.39 (m, 2H), 7.56 (ddd, *J* = 1.4, 7.9, 11.9 Hz, 1H), 7.91 (ddd, *J* = 1.2, 5.9, 13.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 18.3 (*C*H$_3$), 18.7 (*C*H$_3$), 19.7 (d, *J* = 2.9 Hz, *C*H$_3$), 21.8 (d, *J* = 3.9 Hz, *C*H$_3$), 22.0 (d, *J* = 3.8 Hz, *C*H$_3$), 25.0 (*C*H$_3$), 25.1 (*C*H$_3$), 37.6 (d, *J* = 4.8 Hz, *C*H), 49.8 (br, B-*C*), 84.1 (*C*), 124.9 (d, *J* = 13.4 Hz, *C*H), 125.1 (d, *J* = 13.5 Hz, *C*H), 131.2 (d, *J* = 2.9 Hz, *C*H), 131.3 (d, *J* = 2.0 Hz, *C*H), 131.5 (d, *J* = 11.5 Hz, *C*H), 131.7 (d, *J* = 11.5 Hz, *C*H), 132.9 (d, *J* = 11.5 Hz, *C*H), 133.6 (d, *J* = 25.9 Hz, *C*), 133.7 (d, *J* = 10.5 Hz, *C*H), 134.8 (d, *J* = 27.8 Hz, *C*), 141.9 (d, *J* = 9.6 Hz, *C*), 142.1 (d, *J* = 9.6 Hz, *C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 33.1. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 27.2. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{25}H_{37}{}^{11}BNO_3PNa$, 464.2501; found, 464.2501. $[\alpha]_D^{27.4}$ +1.44 (*c* 1.08 in $CHCl_3$, 97% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 9.57 min., *R* isomer: t_R = 10.16 min. IR (neat, cm^{-1}): 1191 (P=O).

(*R*)-*N*-[3,3-Dimethyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butan-2-yl]-*P*,*P*-di-*o*-tolylphosphinic amide [(*R*)-3e].

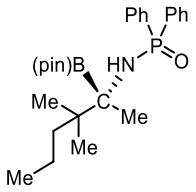


(*R*)-**3e**

The reaction was conducted with 63.6 mg (0.20 mmol) of **1e** for 20 h. The product (*R*)-**3e** was purified by flash column chromatography (SiO_2, CH_2Cl_2/Et_2O, 100:0→80:20) and obtained in 85% yield (74.9 mg, 0.16 mmol, white solid) with 99% ee.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.04 (s, 9H), 1.28 (s, 6H), 1.29 (s, 6H), 1.37 (s, 3H), 2.40 (s, 3H), 2.50 (s, 3H), 2.77 (d, *J* = 9.4 Hz, 1H), 7.15–7.24 (m, 4H), 7.34 (tq, *J* = 1.4, 7.8 Hz, 2H), 7.66 (ddd, *J* = 1.3, 7.8, 15.7 Hz, 1H), 7.94 (ddd, *J* = 1.4, 7.8, 11.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 18.0 (d, *J* = 2.9 Hz *C*H_3), 21.86 (d, *J* = 2.9 Hz, *C*H_3), 21.94 (d, *J* = 3.8 Hz, *C*H_3), 25.0 (*C*H_3), 25.2 (*C*H_3), 26.5 (*C*H_3), 37.2 (d, *J* = 4.7 Hz, *C*), 52.7 (br, B-*C*), 84.2 (*C*), 124.6 (d *J* = 12.5 Hz, *C*H), 125.1 (d, *J* = 13.4 Hz, *C*H), 131.1 (d, *J* = 2.9 Hz, *C*H), 131.2 (d, *J* = 2.9 Hz, *C*H), 131.5 (d, *J* = 7.7 Hz, *C*H), 131.6 (d, *J* = 7.7 Hz, *C*H), 132.9 (d, *J* = 10.5 Hz, *C*H), 133.5 (d, *J* = 10.5 Hz, *C*H), 133.9 (d, *J* = 28.8 Hz, *C*), 135.1 (d, *J* = 29.7 Hz, *C*), 141.5 (d, *J* = 9.5 Hz, *C*), 142.1 (d, *J* = 10.6 Hz, *C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 33.3. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 26.9. HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{26}H_{40}{}^{11}BNO_3P$, 456.2839; found, 456.2831. $[\alpha]_D^{23.3}$ −11.68 (*c* 1.01 in $CHCl_3$, 99% ee). Daicel CHIRALPAK® IA-3, 2-PrOH/Hexane = 8/92, 0.5 mL/min, 40 °C, *S* isomer: t_S = 48.21 min., *R* isomer: t_R = 51.56 min. mp 114–120 °C. IR (neat, cm^{-1}): 1191 (P=O).

(*R*)-*N*-[3,3-Dimethyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexan-2-yl]-*P*,*P*-diphenylphosphinic amide [(*R*)-3f].



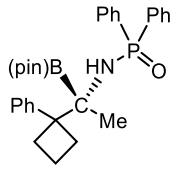
(*R*)-**3f**

The reaction was conducted with 64.8 mg (0.20 mmol) of **1f** for 3 h. The product (*R*)-**3f** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→50:50) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3f** was obtained in 82% yield (73.9 mg, 0.16 mmol, colorless oil) with 99% ee.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.91 (t, *J* = 6.9 Hz, 3H), 0.955 (s, 3H), 0.961 (s, 3H), 1.17 (s, 3H), 1.21–1.48 (m, 4H), 1.28 (s, 6H), 1.32 (s, 6H), 3.07 (d, *J* = 7.4 Hz, 1H), 7.38–7.48 (m, 6H), 7.79–7.89 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 15.3 (*C*H_3), 16.8 (d, *J* = 4.8 Hz *C*H_3), 17.7 (*C*H_2), 22.0 (d, *J* = 28.4 Hz, *C*H_3), 25.0 (*C*H_3), 25.1 (*C*H_3), 39.3 (d, *J* = 4.8 Hz, *C*), 39.9 (*C*H_2), 53.5 (br, B-*C*), 128.3 (*C*H), 128.4 (*C*H), 131.19 (d, *J* = 2.8 Hz, *C*H), 131.23 (d, *J* = 2.9 Hz, *C*H), 131.7 (d, *J* = 9.4 Hz, *C*H), 131.9 (d, *J* = 9.4 Hz, *C*H), 135.5 (*C*), 136.8 (d, *J* = 5.6 Hz, *C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 33.7. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 22.5. HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{26}H_{40}{}^{11}BNO_3P$, 456.2838; found, 456.2834. $[\alpha]_D^{27.9}$ +2.15 (*c* 0.93 in $CHCl_3$, 99% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 9.39 min., *R* isomer: t_R = 12.77 min. IR

(neat, cm^{-1}): 1199 (P=O).

(*R*)-*P*,*P*-Diphenyl-*N*-[1-(1-phenylcyclobutyl)-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phosphinic amide [(*R*)-3g].

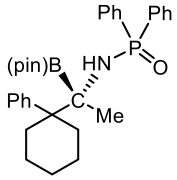


(*R*)-**3g**

The reaction was conducted with 74.2 mg (0.20 mmol) of **1g** for 2 h. The product (*R*)-**3g** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→0:100) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3g** was obtained in 74% yield (73.4 mg, 0.15 mmol, colorless oil) with 98% ee.

^1H NMR (396 MHz, $CDCl_3$, δ): 1.09 (s, 3H), 1.30 (s, 6H), 1.34 (s, 6H), 1.75–1.89 (m, 2H), 2.37–2.44 (m, 2H), 2.67–2.74 (m, 1H), 2.77–2.84 (m, 1H), 2.88 (d, *J* = 5.5 Hz, 1H), 7.20–7.48 (m, 13H), 7.78–7.83 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 15.5 (*C*H_2), 17.7 (d, *J* = 3.8 Hz, *C*H_3), 25.3 (*C*H_3), 30.4 (d, *J* = 31.1 Hz, *C*H_2), 51.8 (br, B-*C*), 52.6 (d, *J* = 6.5 Hz, *C*), 84.3 (*C*), 125.9 (*C*H), 127.3 (*C*H), 128.1 (d, *J* = 12.3 Hz, *C*H), 128.3 (d, *J* = 13.3 Hz, *C*H), 128.9 (*C*H), 131.1 (d, *J* = 1.9 Hz, *C*H), 131.2 (d, *J* = 2.8 Hz, *C*H), 131.7 (d, *J* = 9.5 Hz, *C*H), 135.3 (d, *J* = 34.0 Hz, *C*), 136.6 (d, *J* = 28.3 Hz, *C*), 147.1 (*C*). $^{11}B\{^1H\}$ NMR (127 MHz, $CDCl_3$, δ): 32.7. $^{31}P\{^1H\}$ NMR (159 MHz, $CDCl_3$, δ): 22.4. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{30}H_{37}{}^{11}BNO_3PNa$, 524.2502; found, 524.2501. $[\alpha]_D^{28.0}$ +1.67 (*c* 1.50 in $CHCl_3$, 98% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 10.85 min., *R* isomer: t_R = 15.55 min. IR (neat, cm^{-1}): 1200 (P=O).

(*R*)-*P*,*P*-Diphenyl-*N*-[1-(1-phenylcyclohexyl)-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl]phosphinic amide [(*R*)-3h].



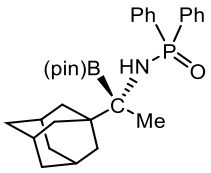
(*R*)-**3h**

The reaction was conducted with 79.4 mg (0.20 mmol) of **1h** for 3 h. The product (*R*)-**3h** was purified by flash column chromatography (SiO_2, CH_2Cl_2/EtOAc, 100:0→90:10 to SiO_2, EtOAc

/MeOH, 100:0→50:50) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. . After filtration, (*R*)-**3h** was obtained in 72% yield (75.3 mg, 0.14 mmol, white solid) with 97% ee.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.06 (s, 3H), 1.13–1.26 (m, 3H), 1.30 (s, 6H), 1.33 (s, 6H), 1.50–1.60 (m, 4H), 1.73 (t, *J* = 13.1 Hz, 1H), 2.55 (t, *J* = 13.3 Hz, 2H), 2.93 (d, *J* = 3.9 Hz, 1H), 7.19 (td, *J* = 3.1, 7.6 Hz, 2H), 7.27–7.45 (m, 11H), 7.77 (ddd, *J* = 1.5, 7.8, 11.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 18.0 (d, *J* = 3.9 Hz, *C*H$_3$), 22.5 (d, *J* = 2.8 Hz, *C*H$_2$), 25.0 (*C*H$_3$), 25.2 (*C*H$_3$), 26.9 (*C*H$_2$), 31.5 (d, *J* = 70.9 Hz, *C*H$_2$), 48.8 (d, *J* = 6.7 Hz, *C*), 53.8 (br, B-*C*), 84.3 (*C*), 125.8 (*C*H), 127.8 (*C*H), 128.0 (d, *J* = 13.4 Hz, *C*H), 128.3 (d, *J* = 12.5 Hz, *C*H), 130.0 (*C*H), 130.9 (d, *J* = 1.9 Hz, *C*H), 131.1 (d, *J* = 1.9 Hz, *C*H), 131.5 (d, *J* = 9.6 Hz, *C*H), 131.7 (d, *J* = 9.6 Hz, *C*H), 135.5 (d, *J* = 38.3 Hz, *C*), 136.7 (d, *J* = 32.6 Hz, *C*), 140.7 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 32.9. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 22.7. HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{32}H_{42}{}^{11}BNO_3P$, 530.2996; found, 530.2998. $[\alpha]_D^{27.9}$ +0.48 (*c* 1.05 in $CHCl_3$, 97% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 9.92 min., *R* isomer: t_R = 12.13 min. mp 79–81 °C. IR (neat, cm^{-1}): 1196 (P=O).

***N*-{(*R*)-1-[(3*R*,5*R*,7*R*)-Adamantan-1-yl]-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl}-*P*,*P*-diphenylphosphinic amide [(*R*)-3i].**



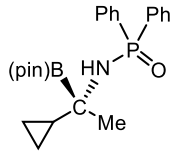
(*R*)-**3i**

The reaction was conducted with 74.2 mg (0.20 mmol) of **1i** for 5 h. The product (*R*)-**3i** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→20:80) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3i** was obtained in 87% yield (86.8 mg, 0.17 mmol, white solid) with 99% ee.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 1.14 (s, 3H), 1.30 (s, 6H), 1.33 (s, 6H), 1.60–1.77 (m, 12H), 2.02 (s, 3H), 3.05 (d, *J* = 7.9 Hz, 1H), 7.38–7.48 (m, 6H), 7.80–7.88 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 15.5 (d, *J* = 4.8 Hz *C*H$_3$), 25.1 (*C*H$_3$), 25.2 (*C*H$_3$), 28.8 (*C*H), 37.35 (*C*H$_2$), 37.44 (*C*H$_2$), 38.3 (d, *J* = 4.8 Hz, *C*), 53.0 (br, B-*C*), 84.3 (*C*), 128.3 (d, *J* = 1.9 Hz, *C*H), 128.4 (d, *J* = 1.9 Hz, *C*H), 131.16 (d, *J* = 2.9 Hz, *C*H), 131.23 (d, *J* = 1.9 Hz, *C*H), 131.7 (d, *J* = 9.6 Hz, *C*H), 132.0 (d, *J* = 9.6 Hz, *C*H), 135.7 (d, *J* = 3.8 Hz, *C*H), 137.0 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 33.7. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 22.5. HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{30}H_{42}{}^{11}BNO_3P$, 506.2995; found,

506.2989. $[\alpha]_D^{27.8}$ −1.34 (*c* 1.12 in $CHCl_3$, 99% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 11.28 min., *R* isomer: t_R = 13.47 min. mp 194–197 °C. IR (neat, cm^{-1}): 1202 (P=O).

(*R*)-*N*-[1-Cyclopropyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl]-*P*,*P*-diphenylphosphinic amide [(*R*)-3j].

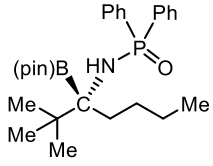


(*R*)-**3j**

The reaction was conducted with 56.3 mg (0.20 mmol) of **1j** for 2 h. The product (*R*)-**3j** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→20:80) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3j** was obtained in 50% yield (40.5 mg, 0.10 mmol, colorless oil) with 86% ee.

^1H NMR (392 MHz, $CDCl_3$, δ): 0.29–0.32 (m, 2H), 0.34–0.46 (m, 2H), 1.04–1.14 (m, 1H), 1.24 (s, 3H), 1.25 (s, 6H), 1.26 (s, 6H), 3.08 (d, *J* = 8.6 Hz, 1H), 7.38–7.48 (m, 6H), 7.82–7.90 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 1.93 (*C*H_2), 2.56 (*C*H_2), 21.6 (d, *J* = 5.6 Hz, *C*H), 22.9 (d, *J* = 3.8 Hz, *C*H_3), 24.8 (*C*H_3), 24.9 (*C*H_3), 84.3 (*C*), 128.2 (d, *J* = 2.9 Hz, *C*H), 128.4 (d, *J* = 3.8 Hz, *C*H), 131.29 (*C*H), 131.31 (*C*H), 131.9 (d, *J* = 9.6 Hz, *C*H), 132.0 (d, *J* = 8.5 Hz, *C*H), 135.1 (*C*), 136.4 (*C*). The carbon directly attached to the boron atom was not detected, likely because of quadrupolar relaxation. $^{11}B\{^1H\}$ NMR (127 MHz, $CDCl_3$, δ): 33.0. $^{31}P\{^1H\}$ NMR (159 MHz, $CDCl_3$, δ): 22.2. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{23}H_{31}{}^{11}BNO_3PNa$, 434.2031; found, 434.2029. $[\alpha]_D^{25.2}$ −2.44 (*c* 1.17 in $CHCl_3$, 86% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 21.95 min., *R* isomer: t_R = 28.56 min. IR (neat, cm^{-1}): 1197 (P=O).

(*R*)-*N*-[2,2-Dimethyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)heptan-3-yl]-*P*,*P*-diphenylphosphinic amide [(*R*)-3k].

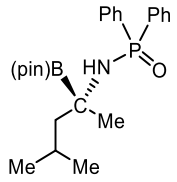


(*R*)-**3k**

The reaction was conducted with 67.2 mg (0.20 mmol) of **1k** for 2 h. The product (*R*)-**3k** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→20:80) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3k** was obtained in 80% yield (73.6 mg, 0.16 mmol, colorless oil) with 86% ee.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.63 (t, *J* = 7.3 Hz, 3H), 0.84–1.21 (m, 4H), 1.03 (s, 9H), 1.25 (s, 6H), 1.26 (s, 6H), 1.62 (dt, *J* = 6.5, 18.8 Hz, 1H), 1.82–1.94 (m, 1H), 3.04 (d, *J* = 11.0 Hz, 1H), 7.37–7.46 (m, 6H), 7.73–7.79 (m, 2H), 7.86–7.91 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H$_3$), 23.5 (*C*H$_2$), 25.0 (*C*H$_3$), 25.2 (*C*H$_3$), 27.3 (*C*H$_3$), 29.7 (*C*H$_2$), 31.3 (d, *J* = 2.8 Hz, *C*H$_2$), 37.9 (*C*), 60.0 (br, B-*C*), 84.4 (*C*), 128.0 (d, *J* = 13.2 Hz, *C*H), 128.3 (d, *J* = 12.3 Hz, *C*H), 130.9 (d, *J* = 2.9 Hz, *C*H), 131.0 (d, *J* = 1.9 Hz, *C*H), 131.3 (d, *J* = 10.4 Hz, *C*H), 132.2 (d, *J* = 10.4 Hz, *C*H), 136.6 (d, *J* = 61.4 Hz, *C*), 137.9 (d, *J* = 59.5 Hz, *C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 33.0. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 22.2. HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{27}H_{42}{}^{11}BNO_3P$, 470.2995; found, 470.2989. $[\alpha]_D^{25.7}$ +1.40 (*c* 3.67 in $CHCl_3$, 88% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 9.49 min., *R* isomer: t_R = 12.08 min. IR (neat, cm^{-1}): 1204 (P=O).

(*R*)-*N*-[4-Methyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentan-2-yl]-*P*,*P*-diphenylphosphinic amide [(*R*)-3l].

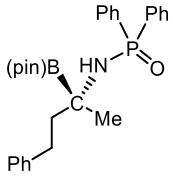


(*R*)-**3l**

The reaction was conducted with 60.2 mg (0.20 mmol) of **1i** for 2 h. The product (*R*)-**3i** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→40:60) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3l** was obtained in 86% yield (73.5 mg, 0.17 mmol, colorless oil) with 88% ee.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.90 (d, *J* = 6.7, Hz, 3H), 0.93 (d, *J* = 6.7, Hz, 3H), 1.23 (s, 3H), 1.26 (s, 6H), 1.28 (s, 6H), 1.44 (dd, *J* = 7.6, 13.9 Hz, 1H), 1.68 (dd, *J* = 5.5, 13.3 Hz, 1H), 1.83–1.97 (m, 1H), 3.11 (d, *J* = 9.0 Hz, 1H), 7.39–7.50 (m, 6H), 7.77–7.83 (m, 2H), 7.87–7.93 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 23.7 (*C*H_3), 24.2 (*C*H_3), 24.6 (d, *J* = 4.8 Hz, *C*H_3), 25.0 (*C*H_3), 25.3 (*C*H), 45.7 (br, B-*C*), 50.6 (d, *J* = 2.9 Hz, *C*H_2), 84.4 (*C*), 128.3 (d, *J* = 3.8 Hz, *C*H), 128.4 (d, *J* = 3.8 Hz, *C*H), 131.3 (*C*H), 131.7 (d, *J* = 9.5 Hz, *C*H), 132.1 (d, *J* = 9.4 Hz, *C*H), 135.2 (*C*), 136.5 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 33.8. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 21.9. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{24}H_{35}{}^{11}BNO_3P$, 450.2344; found, 450.2340. $[\alpha]_D^{25.9}$ +1.34 (*c* 4.28 in $CHCl_3$, 88% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 13.73 min., *R* isomer: t_R = 17.52 min. IR (neat, cm^{-1}): 1198 (P=O).

(*R*)-*P*,*P*-Diphenyl-*N*-[4-phenyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butan-2-yl]phosphinic amide [(*R*)-3m].

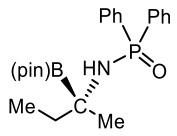


(R)-**3m**

The reaction was conducted with 69.1 mg (0.20 mmol) of **1m** for 6 h. The product (*R*)-**3m** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→40:60) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3m** was obtained in 44% yield (41.4 mg, 0.09 mmol, colorless oil) with 89% ee.

^{1}H NMR (392 MHz, $CDCl_3$, δ):1.285–1.294 (m, 15H), 1.82 (td, *J* = 4.3, 12.9 Hz, 1H), 2.00 (td, *J* = 5.0, 13.0 Hz, 1H), 2.57 (td, *J* = 4.7, 12.9 Hz, 1H), 2.87 (td, *J* = 4.8, 12.9 Hz, 1H), 3.21 (d, *J* = 8.6 Hz, 1H), 7.13–7.16 (m, 3H), 7.23–7.27 (m, 2H), 7.39–7.52 (m, 6H) , 7.83–7.92 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 24.2 (d, *J* = 3.8 Hz, *C*H_3), 24.9 (*C*H_3), 25.0 (*C*H_3), 32.3 (*C*H_2), 43.5 (d, *J* = 3.8 Hz, *C*H_2), 46.1 (br, B-*C*), 84.5 (*C*), 125.8 (*C*H), 128.3 (d, *J* = 2.9 Hz, *C*H), 128.40 (*C*H), 128.45 (d, *J* = 1.9 Hz, *C*H), 128.55 (*C*H), 135.0 (d, *J* = 5.7 Hz, *C*), 136.3 (d, *J* = 6.6 Hz, *C*), 142.7 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 32.6. ^{31}P{^{1}H} NMR (159 MHz, $CDCl_3$, δ): 22.1. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{28}H_{35}{}^{11}BNO_3PNa$, 498.2345; found, 498.2339. $[\alpha]_D^{22.0}$ –13.9 (*c* 0.85 in $CHCl_3$, 89% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 5/95, 0.5 mL/min, 40 °C, *S* isomer: t_S = 32.80 min., *R* isomer: t_R = 47.56 min. IR (neat, cm^{-1}): 1196 (P=O).

(*R*)-*P*,*P*-Diphenyl-*N*-[2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butan-2-yl]phosphinic amide [(*R*)-3n].

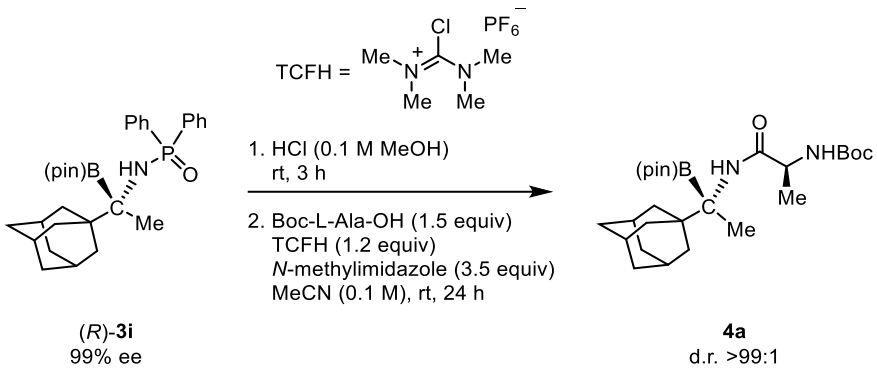


(*R*)-**3n**

The reaction was conducted with 53.8 mg (0.20 mmol) of **1n** for 1 h. The product (*R*)-**3n** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→50:50) and extracted with H_2O to remove pinacol, and dried over $MgSO_4$. After filtration, (*R*)-**3n** was obtained in 28% yield (22.3 mg, 0.06 mmol, colorless oil) with 69% ee.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.94 (t, *J* = 7.4 Hz, 3H), 1.23 (s, 3H), 1.26 (s, 6H), 1.27 (s, 6H), 1.57 (sxt, *J* = 7.2 Hz, 1H), 1.70 (sxt, *J* = 7.1 Hz, 1H), 3.11 (d, *J* = 9.0 Hz, 1H), 7.39–7.49 (m, 6H), 7.82–7.91 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 10.1 (*C*H$_3$), 23.6 (d, *J* = 3.8 Hz, *C*H$_3$), 24.9 (*C*H$_3$), 25.0 (*C*H$_3$), 34.2 (d, *J* = 3.8 Hz, *C*H$_2$), 46.7 (br, B-*C*), 84.3 (*C*), 128.2 (*C*H), 128.4 (*C*H), 131.3 (*C*H), 131.8 (d, *J* = 10.4 Hz, *C*H), 132.1 (d, *J* = 10.4 Hz, *C*H), 135.1 (*C*), 136.4 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 32.5. ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$, δ): 22.0. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{22}H_{31}{}^{11}BNO_3P$,422.2031; found, 422.2026. $[\alpha]_D^{25.0}$ +18.9 (*c* 0.12 in $CHCl_3$, 69% ee). Daicel CHIRALPAK® OZ-3, 2-PrOH/Hexane = 10/90, 0.5 mL/min, 40 °C, *S* isomer: t_S = 19.49 min., *R* isomer: t_R = 24.40 min. IR (neat, cm^{-1}): 1196 (P=O).

4. Experimental Procedures for the Synthesis of Peptydilboronic Acid Derivatives

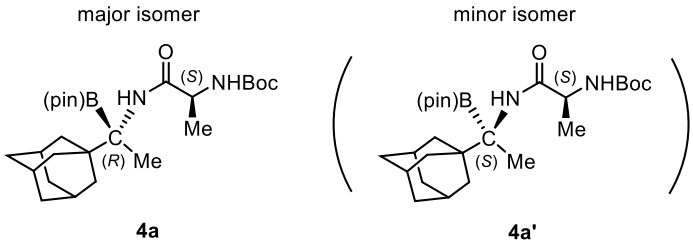


(*R*)-**3i**
99% ee

4a
d.r. >99:1

The borylation product (*R*)-**3i** (177 mg, 0.35 mmol, 1.0 equiv) was placed in a vial with a screw cap containing a Teflon®-coated rubber septum under air. A MeOH solution of HCl (0.1 M, 3.5 mL) was added to the vial via a syringe. The resulting mixture was stirred for 3 h at room temperature. The solvents are removed under reduced pressure to afford the deprotection product. The product was used in the next step without further purification. The condensation reaction was performed according to the literature.[7]. Boc-L-Ala-OH (85.9 mg, 0.46 mmol, 1.3 equiv) and TCFH (118 mg, 0.42 mmol, 1.2 equiv) were placed in a vial with a screw cap containing a Teflon®-coated rubber septum under air. MeCN (100 μL) was added to the vial via a syringe. The resulting mixture was stirred for 5 min at room temperature. A THF solution (250 μL) of the deprotection product was then added dropwise to the vial. *N*-Metylimidazole (94 μL, 1.2 mmol, 3.5 equiv) was added dropwise to the vial. The reaction mixture was stirred for 24 h. The reaction mixture was analyzed by TLC to check the completeness of the reaction. The mixture was directly filtered through a short silica-gel column with EtOAc as an eluent, then the resultant solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane/EtOAc eluent (100:0 to 40:60) to give the corresponding product **4a** in 71% yield (118.0 mg, 0.25 mmol) as white solid. The diastereomeric ratio was determined by HPLC analysis (d.r. >99:1).

***tert*-Butyl [(*S*)-1-({(*R*)-1-[(3*R*,5*R*,7*R*)-adamantan-1-yl]-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl}amino)-1-oxopropan-2-yl]carbamate (4a).**



4a **4a'**

NMR spectra for **4a** contains conformational isomers, which is caused by the restricted C−N bond rotation around the carbamate group. ^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.14 (s, 3H), 1.23 (s, 6H), 1.24 (s, 6H), 1.35 (d, *J* = 7.4 Hz, 3H), 1.45 (s, 9H), 1.60–1.76 (m, 12H), 1.96 (s, 3H), 4.09–4.29 (m, 1H), 4.73–5.01 (m, 1H), 6.59–6.87 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 16.4 (*C*H_3), 24.9 (*C*H_3), 25.2 (*C*H_3), 25.5 (*C*H_3), 28.4 (*C*H_3), 28.7 (*C*H), 36.9 (*C*H_2), 37.2 (*C*H_2), 37.5 (*C*), 48.0 (*C*H), 51.1 (br, B-*C*), 75.1 and 80.5 (a pair of s, *C*), 81.9 (*C*), 155.8 (*C*), 173.8 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 25.5. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{26}H_{45}N_2O_5{}^{11}BNa$, 499.3319; found, 499.3313. $[\alpha]_D^{22.3}$ –25.3 (*c* 0.39 in $CHCl_3$). The diastereomeric ratio was determined by HPLC analysis (d.r. >99:1, right side in Figure S1) by comparison with a mixture of the diastereomers that was obtained by the reaction of racemic **3i** with Boc-L-Ala-OH (d.r. 80:20, left side in Figure S1). Daicel CHIRALPAK® ID-3, 2-PrOH/Hexane = 3/97, 0.5 mL/min, 40 °C, minor isomer = 11.88 min., major isomer = 15.07 min. mp 82–92 °C. IR (neat, cm^{-1}): 1699 (C=O, amide).

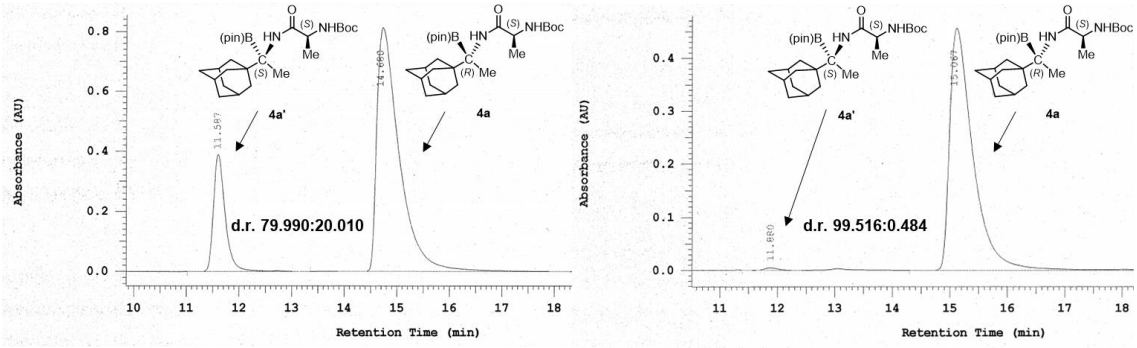
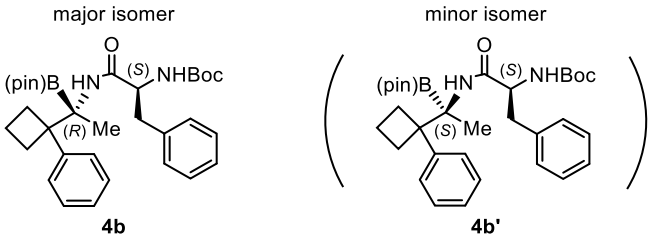


Figure S1. Determination of the diastereomeric ratio of **4a** by HPLC analysis.

***tert*-Butyl ((*S*)-1-oxo-3-phenyl-1-{[(*R*)-1-(1-phenylcyclobutyl)-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl]amino}propan-2-yl)carbamate (4b).**



4b was synthesized according to the procedure for the synthesis of **4a**. The reaction was conducted with 100.5 mg (0.20 mmol) of (*R*)-**3g** using Boc-L-Phe-OH (79.9 mg, 0.30 mmol, 1.5 equiv) and TCFH (78.2 mg, 0.28 mmol, 1.4 equiv). The product **4b** was purified by flash column chromatography (SiO_2, hexane/EtOAc, 100:0→70:30) to give the corresponding product **4b** in 62% yield (69.3 mg, 0.12 mmol) as white solid. The diastereomeric ratio was determined by HPLC analysis (d.r. >99:1).

NMR spectra for **4b** contains conformational isomers, which is caused by the restricted C−N bond rotation around the carbamate group. ^{1}H NMR (396 MHz, $CDCl_3$, δ): 0.82 (brs, 3H), 1.29 (s, 6H), 1.35 (s, 6H), 1.35–1.39 (m, 9H), 1.66–1.85 (m, 2H), 2.16–2.23 (m, 1H), 2.34–2.42 (m, 1H), 2.50–2.58 (m, 1H), 2.72–2.84 (m, 1H), 2.94 (dd, *J* = 6.9, 13.7 Hz, 1H), 3.13 (dd, *J* = 6.1, 14.1 Hz, 1H), 4.23–4.33 (m, 1H), 4.88–4.97 (m, 1H), 5.75–5.86 (m, 1H), 7.12–7.31 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 15.3 (*C*H_2), 18.6 (*C*H_3), 25.4 (*C*H_3), 25.8 (*C*H_3), 28.3 (*C*H_3), 31.0 (*C*H_2), 38.2 (*C*H_2), 48.8 (br, B-*C*), 51.0 (*C*), 54.7 (*C*H), 80.2 (*C*), 82.9 (*C*), 126.0 (*C*H), 127.0 (*C*H), 127.6 (*C*H), 128.6 (*C*H), 128.7 (*C*H), 129.6 (*C*H), 136.4 (*C*), 145.9 (*C*), 155.2 (*C*), 171.8 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 29.1. HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{32}H_{45}N_2O_5{}^{11}BNa$, 571.3319; found, 571.3316. $[\alpha]_D^{22.0}$ –5.94 (*c* 1.10 in $CHCl_3$). The diastereomeric ratio was determined by HPLC analysis (d.r. >99:1). Daicel CHIRALPAK® ID-3, 2-PrOH/Hexane = 3/97, 0.5 mL/min, 40 °C, minor isomer = 8.65 min., major isomer = 12.01 min. mp 62–70 °C. IR (neat, cm^{-1}): 1708 (C=O, amide).

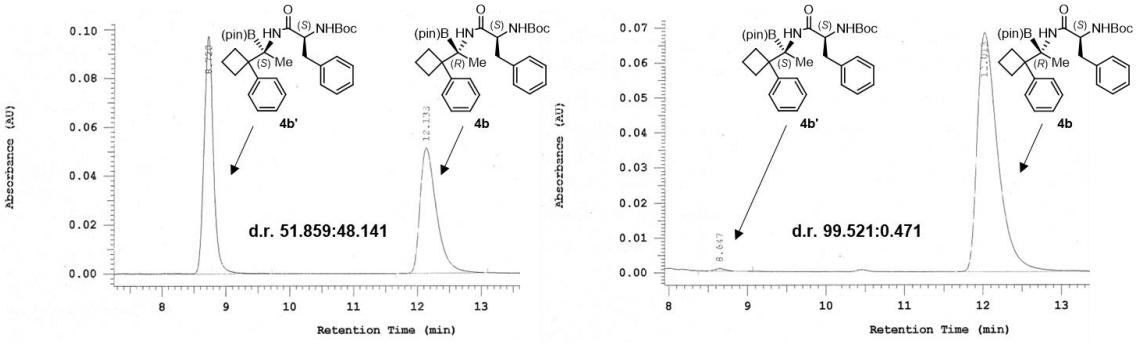
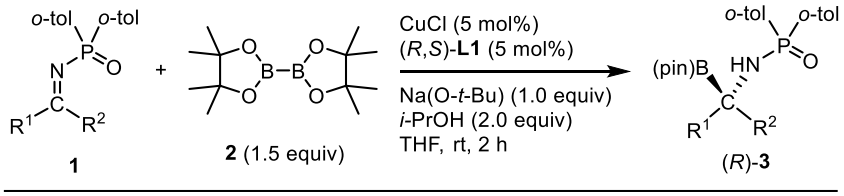
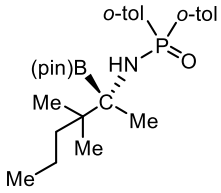


Figure S2. Determination of the diastereomeric ratio of **4b** by HPLC analysis.

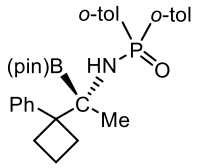
5. Additional Experimental Results

Unsuccessful examples of the borylation of ketimines with P(O)(*o*-tol)$_2$ as the protecting group

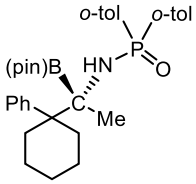




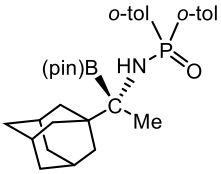
(*R*)-**3f'**
no reaction



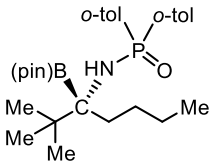
(*R*)-**3g'**
no reaction



(*R*)-**3h'**
no reaction

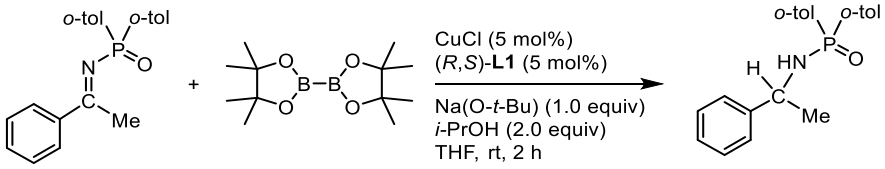


(*R*)-**3i'**
no reaction

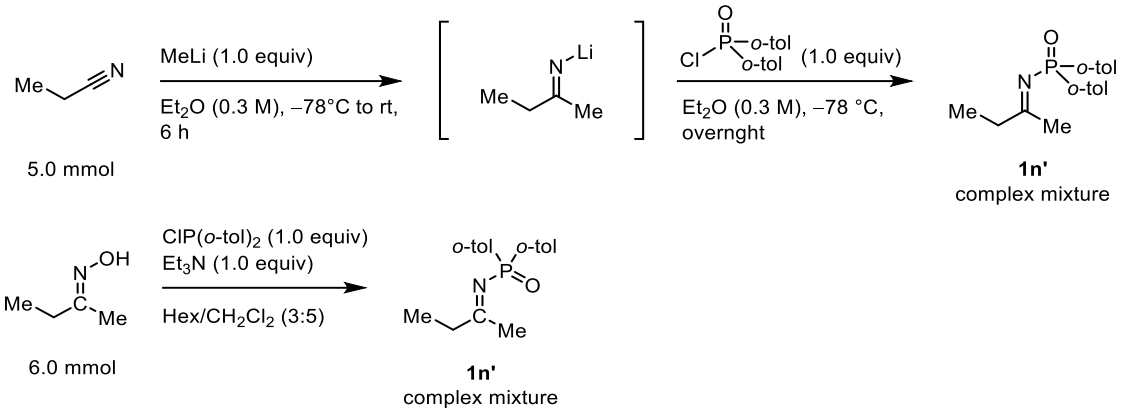


(*R*)-**3k'**
no reaction

An unsuccessful example of the borylation of aromatic ketimine 1o

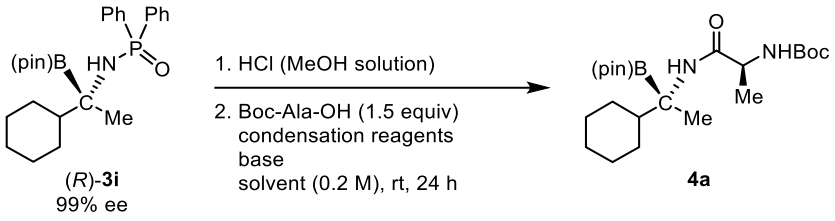


Unsuccessful synthesis of the substrate 1n'

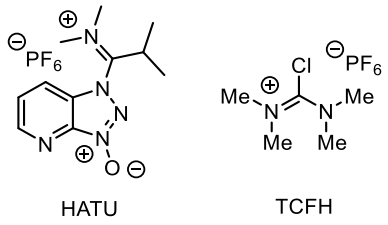


Neither procedure A nor B could synthesize the ketimine **1n'**.

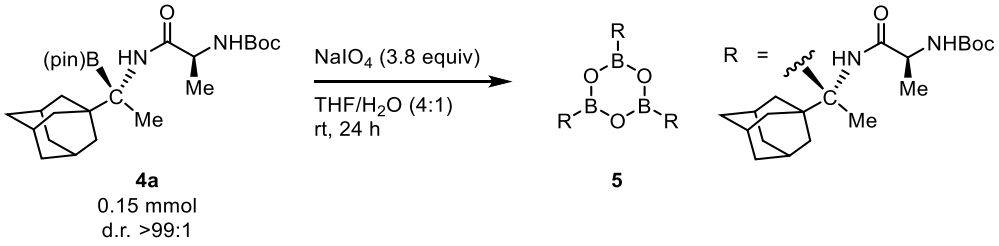
Condensation reactions with Boc-Ala-OH



entry	condensation reagents	base	solvent	yield (%)
1	HATU (3.0 equiv)	*i*-Pr_2EtN (3.0 equiv)	DCM	0
2	TCFH (1.2 equiv)	N-methylimidazole (3.5 equiv)	MeCN	74%



Hydrolysis of 4a with $NaIO_4$



4a (71.6 mg, 0.15 mmol, 1.0 equiv) and $NaIO_4$ (121.9 mg, 0.57 mmol, 3.8 equiv) were placed in a vial with a screw cap containing a Teflon®-coated rubber septum under air. THF (1.0 mL) and H_2O

(250 μL) were added to the vial via a syringe. The resulting mixture was stirred for 24 h at room temperature. The reaction mixture was then diluted with brine and extracted with EtOAc three times, and dried over $MgSO_4$, and concentrated under reduced pressure. The combined mixture was washed cold pentane to give the boroxine **5** in 70% yield (41.3 mg, 0.105 mmol) as white solid. The corresponding boronic acid was not detected.

6. Determination of Absolute Configuration of Borylation Product

The absolute configuration of the product was determined based on X-ray crystallographic analysis of the compound (*R*)-**3e**. The absolute configurations of other borylation products were deduced by this product. The details were summarized in Figure S3 and Table S1.

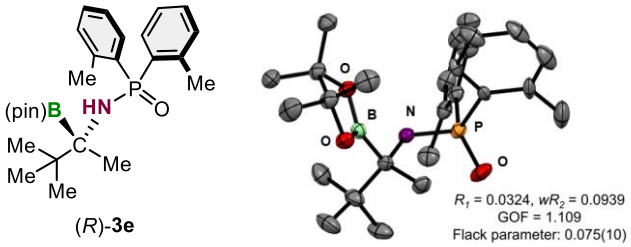


Figure S3. Molecular structure of (*R*)-**3e**. Thermal ellipsoids set at 50% probability; hydrogen atoms omitted for clarity.

Table S1. Summary of X-ray crystallographic data

CCDC Name	2052090
Empirical Formula	$C_{52}H_{78}B_2N_2O_6P_2$
Formula Weight	910.72
Crystal System	monoclinic
Crystal Size / mm^3	0.15 × 0.15 × 0.1
a / Å	7.83470(10)
b / Å	33.8529(3)
c / Å	10.56040(10)
β / °	111.6360(10)
V / Å3	2603.57(5)
Space Group	$P2_1$
Z value	2
*D*calc / g cm^{-3}	1.162
Temperature / K	123
$2\theta_{max}$ / °	147.536
μ(MoKα) /cm^{-1}	11.32
No. of Reflections Measured	Total: 12604 Unique: 7917 (R_{int} = 0.0223)
No. of Observations (All reflections)	7917
Residuals: R_1 (I > 2.00σ(I))	0.0324
Residuals: wR_2 (All reflections)	0.0939
Goodness of Fit Indicator (GOF)	1.109
Maximum Peak in Final Diff. Map / $Å^3$	0.23 e^-
Minimum Peak in Final Diff. Map / $Å^3$	–0.24 e^-
Flack Parameter	0.075(10)

7. Plausible Catalytic Cycle

Based on the theoretical and experimental results, we have proposed a plausible mechanism for the enantioselective borylation of aliphatic ketimines (Figure S4). First, CuCl, (*R*,*S*)-**L1** and Na(O-*t*-Bu) would react to form the copper(I)/NHC complex **A**, which would undergo sigma-bond metathesis with **2** to give borylcopper(I) **B**. The subsequent insertion to **1** would lead to the formation of the copper(I) intermediate **D**, which would be protonated in the presence of an alcohol to afford the borylated product **3**. This step would also result in the formation of copper alkoxide **A**.

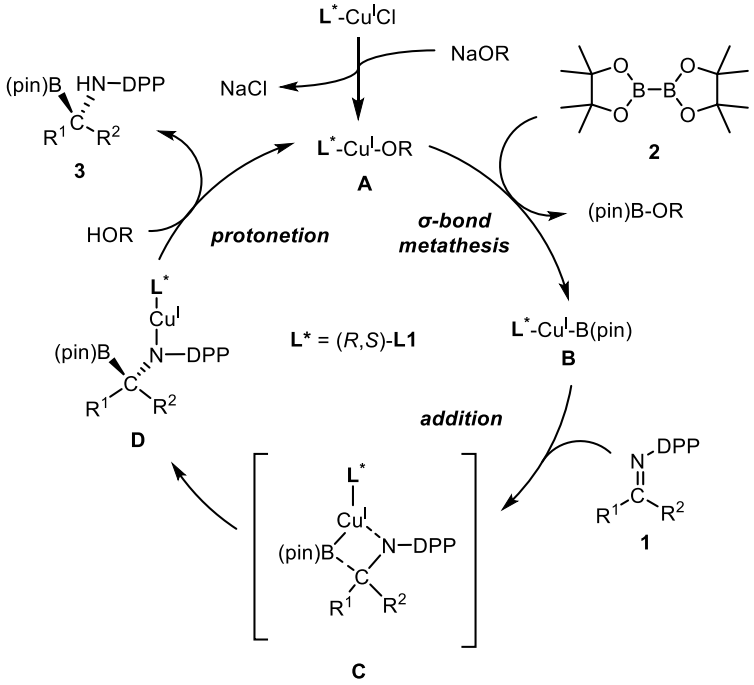
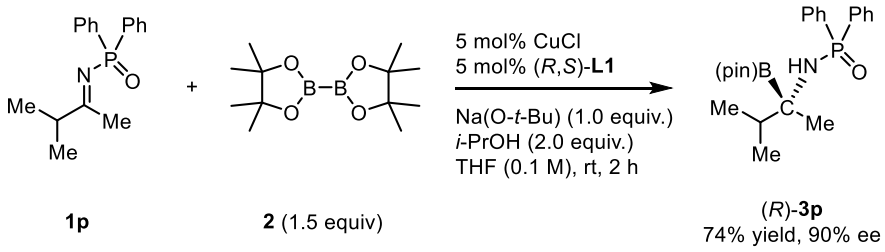


Figure S4. Proposed mechanism for the copper(I)-catalyzed enantioselective borylation of aliphatic ketimines.

8. DFT Calculations

All calculations were performed using the Gaussian 09W (revision C.01) program package.[8] Geometry optimizations and transition states (TS) calculations were performed with wB97XD/def2tzvp//wB97XD/Def2svp/THF(SMD). Molecular structures were drawn using the Mercury 3.5 program.[9] Frequency calculations were conducted on gas-phase optimized geometries to check all the stationary points as either minima or transition states. Intrinsic reaction coordinate (IRC) calculations were carried out to confirm the transition state connecting the correct reactant and product on the potential energy surface.

We conducted the DFT calculations on the addition of the (*R*,*S*)-**L1**/borylcopper(I) complex (**II**) to ketimine **1p** (**I**) to investigate the reaction mechanism and the origin of the enantioselectivity. The copper(I)-catalyzed borylation of dialkyl ketimine **1p** proceeded to give (*R*)-**3p** in 74% yield with 90% ee. As shown in Figure S3, The energy of the transition state (**TS1**) in the *Si*-face addition is lower than that of the transition state (**TS3**) in the *Re*-face addition by 1.93 kcal/mol. This calculation result is in good agreement with the experimental result (calc. 92% ee versus exp. 90% ee).



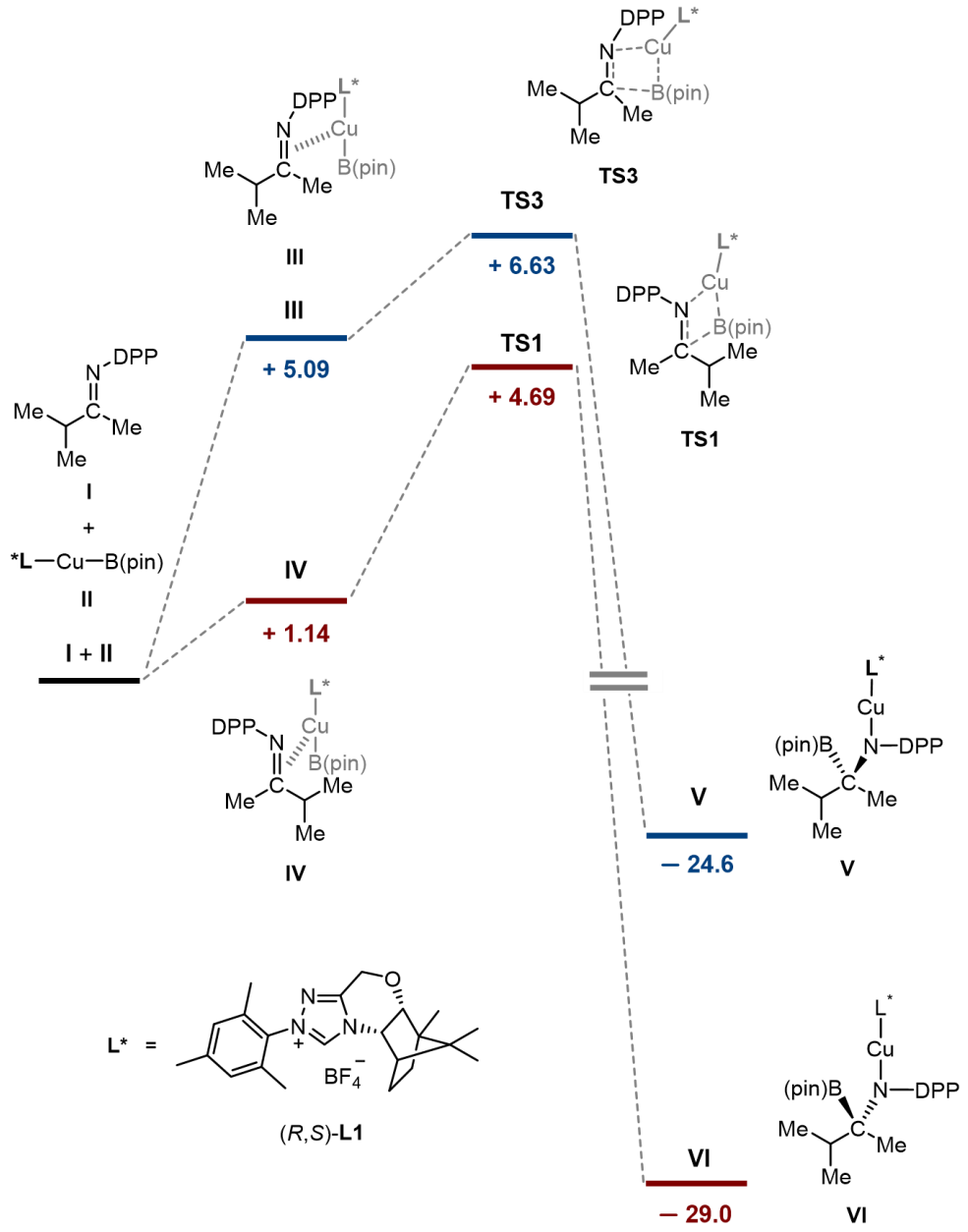


Figure S5. DFT calculations (wB97XD/def2tzvp//wB97XD/Def2svp THF(SMD)) of the addition of the (*R*,*S*)-**L1**/borylcopper(I) complex to ketimine **1p**. Gibbs free energy values relative to **I** and **II** are shown in kcal/mol at 298 K and 1.0 atm in the gas phase.

9. Analysis for Non-Covalent Interactions in the Transition States

Non-covalent interactions (NCIs) in the transition states were computed using the non-covalent interaction index from the optimized electron density at the same level of theory as the geometry optimizations. The wave function files (.wfn) were obtained from the corresponding formatted gaussian checkpoint files (.fchk) using the Multiwfn program.[10] The following thresholds were applied to S33 to generate the NCI plot isosurface with NCIPLOT program,[11,12] sign(λ2)ρ ranging from –0.2 to 0.2 au and reduced density gradient (RDG) = 0.60 au. The surfaces were colored on a blue-green-red (BGR) scale using VMD program[13] according to values of sign(λ2)ρ ranging from –0.01 to 0.01 au. The blue region indicates strong attractive interactions and the red region indicates strong repulsive interactions.

Detailed Analysis of Transition State Structures

The detailed analysis of both transition states **TS1** and **TS3** was carried out by the combination of structural analysis based on the transition state structures and the non-covalent interaction (NCI) plot. As shown in Figure S6, C(sp_3)-H/π interaction between the phenyl group of DPP and the methyl group of the mesityl group was found, and C(sp_3)-H/O interaction between the camphor moiety and an oxygen atom of P=O also existed. These interactions stabilize **TS1** to afford the major enantiomer (*R*)-**3p**. We also performed a non-covalent interaction (NCI) plot analysis of **TS3**. As shown Figure S7, an C(sp_3)-H/π interaction between the phenyl and the methyl group of the mesityl group was found. However, a steric hindrance between the isopropyl group of the substrate (**1p**) and camphor moiety might destabilize **TS3** to produce minor enantiomer (*S*)-**3p**.

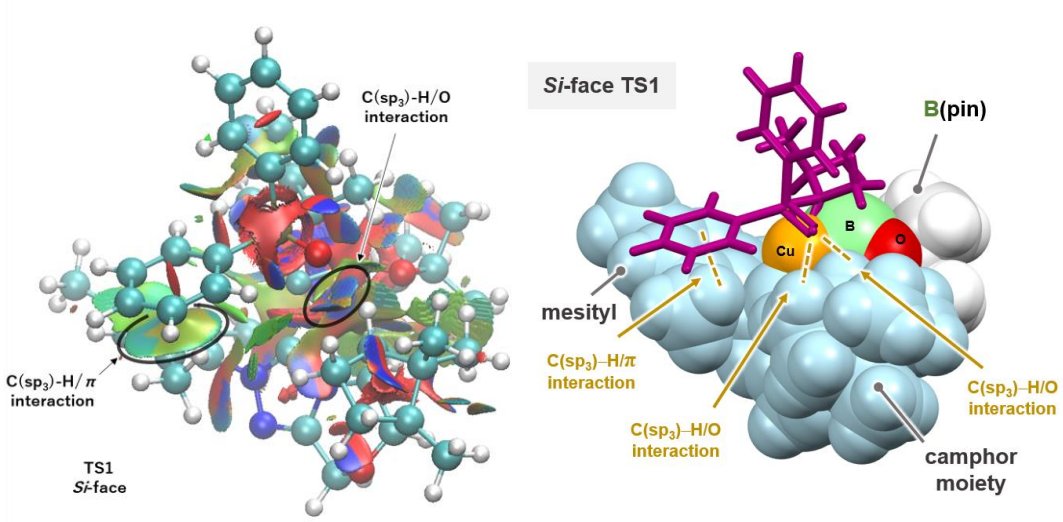


Figure S6. Detailed structural analysis of transition state structure for **TS1**.

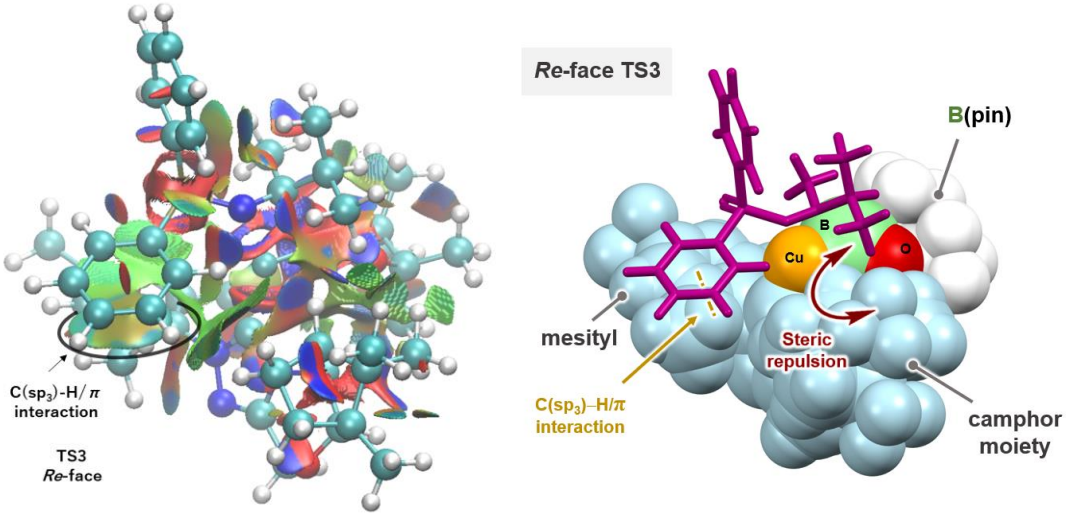
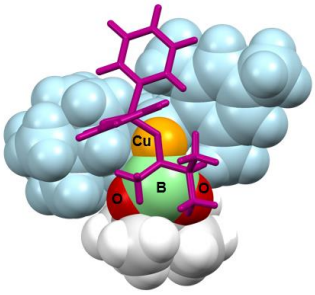


Figure S7. Detailed structural analysis of transition state structure for **TS3**.

Coordination profiles

***Si*-face TS1**



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C	2.87951	-1.15702	3.23617
O	1.29464	0.5591	3.24174
O	2.01939	-1.25353	2.08168
B	1.04317	-0.28889	2.18544
C	-1.0933	-0.96821	1.84609
C	-0.75084	-2.44169	2.04232
C	-1.68923	-0.3093	3.11189
H	-0.9697	-0.47892	3.92995
H	-0.14322	-2.82482	1.21353
N	-1.83164	-0.63708	0.67825
P	-2.18939	-1.61919	-0.58055
O	-1.14826	-2.50003	-1.23821
H	-1.68147	-3.03196	2.07221
H	-0.21208	-2.61301	2.98439
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H	-2.25155	1.64199	3.89294
H	-0.92457	1.69079	2.71302
H	-2.59698	1.42576	2.15807
C	-3.01283	-0.97346	3.5003
H	-3.75729	-0.85034	2.69961
H	-2.90109	-2.05063	3.69406
H	-3.42005	-0.51345	4.41461
C	2.64568	0.3261	3.68469

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H	3.48757	1.16075	1.85083
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H	4.59057	1.23045	3.25488
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H	3.04698	-2.21731	5.13727
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H	4.99762	-1.28291	3.66464
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C	-4.47413	-4.9389	0.18943

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H	0.9258	-0.10712	-2.82631
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C	4.97948	-2.14996	-3.56714
C	-2.47207	4.90357	0.28619
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H	1.96073	-4.30631	-1.4795
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H	5.37879	-1.42285	-4.29172
H	5.78539	-2.3934	-2.85637
C	-3.70785	5.6745	0.66571
H	-3.46886	6.73253	0.8584
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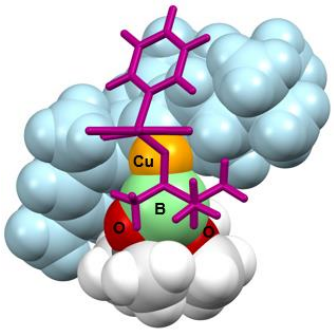
***Si*-face TS2**



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O	-2.91943	1.75152	0.74534
B	-1.8472	1.06861	1.26116
C	0.00828	2.12728	1.09581
C	-0.58113	3.40828	0.5008
C	0.22592	2.24726	2.62941
H	-0.76223	2.4074	3.08942
H	-0.9553	3.24566	-0.51597
N	1.17075	1.62204	0.43376
P	1.81529	2.15062	-0.97157
O	0.93987	2.56239	-2.13733
H	0.21027	4.17287	0.44004
H	-1.39661	3.80546	1.11877
C	0.82759	0.98938	3.24379
H	0.92095	1.09965	4.3356
H	0.19547	0.11143	3.05054
H	1.82951	0.79856	2.83034
C	1.08432	3.46835	2.97296
H	2.064	3.41597	2.47756
H	0.60774	4.41482	2.6795
H	1.25841	3.51316	4.05962
C	-3.60029	0.53551	2.62565

C	-3.9048	0.7004	4.10512
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H	-2.90646	3.19888	3.00589
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C	2.57985	0.09628	-2.67174
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C	3.33966	-0.993	-3.1011
H	1.73442	0.45313	-3.26437
C	4.43533	-1.41957	-2.34997
H	5.62176	-1.08282	-0.57523
H	3.08268	-1.50164	-4.03372
H	5.04073	-2.26307	-2.69108
C	2.97009	3.53167	-0.61436
C	3.01574	4.60534	-1.51083
C	3.8029	3.55108	0.51212
C	3.88277	5.67611	-1.29046
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C	4.67406	4.61709	0.73092

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H	5.39754	6.5179	0.00092
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N	0.37088	-2.31302	-0.95943
N	-1.34851	-1.59058	-1.93319
C	1.51098	-2.53597	-0.08492
C	-0.01044	-3.20012	-1.92444
N	-1.07413	-2.78294	-2.53857
C	-2.57064	-0.90495	-2.22373
C	1.26752	-2.20355	1.39305
C	1.91451	-4.05329	-0.0484
H	2.33978	-1.93429	-0.47718
C	0.74492	-4.4817	-2.04738
C	-3.75288	-1.42717	-1.67415
C	-2.54881	0.25243	-3.0067
C	-0.0052	-2.92562	1.86445
H	1.28865	-1.12419	1.58661
C	2.39702	-3.02299	2.07551
C	1.91038	-4.38001	1.46441
H	2.92652	-4.16895	-0.47449
O	1.04607	-4.91458	-0.74727
H	1.66192	-4.33382	-2.64913
H	0.12628	-5.24313	-2.53777
C	-4.93449	-0.72108	-1.89026
C	-3.73731	-2.70792	-0.88522
C	-3.7607	0.93234	-3.18253
C	-1.27921	0.75168	-3.63347
H	-0.31261	-2.55428	2.85147
H	-0.85731	-2.74941	1.19425
C	0.42979	-4.41194	1.90615

C	3.81816	-2.61484	1.67103
C	2.34097	-2.96062	3.60503
C	2.6989	-5.62801	1.80939
C	-4.9544	0.47021	-2.62766
H	-5.86513	-1.10475	-1.46184
H	-3.52896	-3.56771	-1.54103
H	-2.95361	-2.69523	-0.11189
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H	-3.76499	1.85007	-3.7774
H	-0.65848	1.33408	-2.92962
H	-0.66468	-0.08477	-3.99953
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H	0.34718	-4.836	2.91716
H	-0.16507	-5.0469	1.23801
H	3.99595	-1.55902	1.92871
H	4.55688	-3.21939	2.21976
H	4.03626	-2.72899	0.60227
H	3.09901	-3.62818	4.04357
H	2.56852	-1.93684	3.94242
H	1.36975	-3.23789	4.03384
H	2.69163	-5.81394	2.89455
H	2.2636	-6.51089	1.31589
H	3.74774	-5.544	1.48329
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H	-6.74846	1.39169	-1.85774
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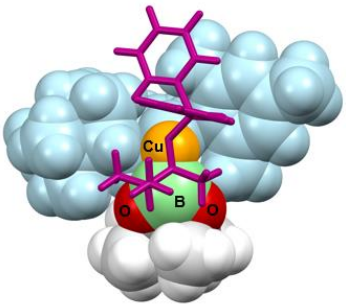
***Re*-face TS3**



Cu	0.00263	-0.39312	0.29451
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C	1.83232	-3.22448	2.82873
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O	2.09154	-2.47938	0.61919
B	0.91833	-1.97684	1.14087
C	-1.01164	-2.13846	0.0175
C	2.29988	-2.91306	4.24125
H	2.58272	-1.85827	4.35433
H	1.48909	-3.12307	4.95437
H	3.16223	-3.54065	4.51321
C	1.22586	-4.62505	2.77261
H	1.94758	-5.39054	3.09213
H	0.35951	-4.66695	3.44892
H	0.8783	-4.87405	1.7592
C	3.89462	-1.86518	2.06939
H	4.56937	-2.17905	2.87863
H	4.51277	-1.63201	1.18954
H	3.37694	-0.94591	2.38249
C	3.65056	-4.20885	1.24363
H	4.37571	-3.93535	0.46292
H	4.20433	-4.66233	2.0796
H	2.96876	-4.96058	0.82517
C	-0.54247	-3.30203	-0.89109
C	-1.83718	-2.63445	1.20427

H	-2.84384	-2.91815	0.85765
H	-1.37263	-3.51133	1.67492
H	-1.96698	-1.85338	1.96213
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H	-0.15099	-2.10497	-2.65868
H	1.28852	-2.41391	-1.64311
H	0.63549	-3.70564	-2.67039
H	0.03207	-3.99981	-0.25816
C	-1.75154	-4.06485	-1.44414
H	-1.4167	-4.88559	-2.09788
H	-2.37064	-4.50763	-0.6507
H	-2.39284	-3.39876	-2.04108
N	-1.55126	-1.04831	-0.7182
P	-2.97752	-0.28642	-0.47111
O	-3.51718	-0.01347	0.91276
C	-4.2424	-1.22675	-1.41343
C	-5.34927	-1.74439	-0.73501
C	-4.10422	-1.47259	-2.78554
C	-6.30107	-2.50751	-1.41434
H	-5.45319	-1.53997	0.33347
C	-5.05785	-2.22558	-3.46708
H	-3.24074	-1.073	-3.32493
C	-6.15649	-2.74833	-2.78018
H	-7.16134	-2.91284	-0.87571
H	-4.94299	-2.41017	-4.53802
H	-6.90234	-3.3426	-3.31399
C	-2.79406	1.26576	-1.41588
C	-1.79963	1.46869	-2.37896
C	-3.70916	2.29103	-1.14979
C	-1.72686	2.67785	-3.07092
H	-1.0732	0.67599	-2.56904
C	-3.64279	3.49592	-1.84802
H	-4.46997	2.13974	-0.37981

C	-2.65164	3.69045	-2.81104
H	-0.94366	2.83071	-3.81775
H	-4.36179	4.29024	-1.63288
H	-2.59445	4.6368	-3.35449
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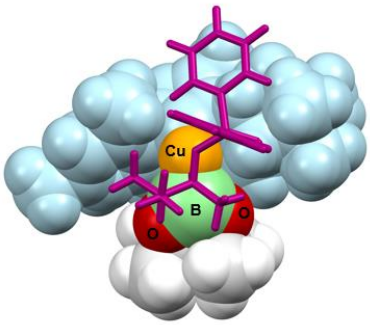
N	2.25213	1.45414	0.35305
N	0.76137	2.16988	1.64932
C	3.04305	0.66262	-0.56743
C	2.71797	2.55731	1.00574
N	1.81463	3.02795	1.81045
C	-0.46767	2.39549	2.34493
C	2.36558	0.31876	-1.89422
C	4.34014	1.41423	-1.00873
H	3.2942	-0.26572	-0.04376
C	4.10077	3.0336	0.69625
C	-1.36785	3.32526	1.80829
C	-0.72595	1.68269	3.52143
C	1.92485	1.61492	-2.59206
H	1.57083	-0.42798	-1.77539
C	3.60299	-0.13141	-2.71811
C	4.32701	1.24942	-2.552
H	5.22499	0.92565	-0.56323
O	4.36283	2.77997	-0.65683
H	4.82995	2.52333	1.35496
H	4.18125	4.1138	0.87062
C	-2.57405	3.52281	2.48162
C	-1.03868	4.06435	0.54208
C	-1.94846	1.91324	4.15751
C	0.27044	0.69857	4.06955
H	1.24092	1.39215	-3.42255
H	1.37656	2.27923	-1.90876
C	3.25912	2.22757	-3.08475
C	4.36556	-1.3275	-2.12795

C	3.25388	-0.50077	-4.16218
C	5.6968	1.40416	-3.18277
C	-2.88446	2.82007	3.6505
H	-3.2945	4.23871	2.076
H	-0.94531	3.36387	-0.30324
H	-1.82231	4.79187	0.29499
H	-0.0818	4.60109	0.6314
H	-2.17534	1.36606	5.07697
H	0.27255	-0.23696	3.48743
H	1.29275	1.10579	4.03986
H	0.03333	0.44348	5.11156
H	3.30901	2.27281	-4.18208
H	3.42698	3.24252	-2.70624
H	3.67901	-2.17447	-1.97568
H	5.15144	-1.6556	-2.82537
H	4.85726	-1.1296	-1.16563
H	4.1697	-0.65209	-4.75468
H	2.69447	-1.44994	-4.17336
H	2.64032	0.2463	-4.6817
H	5.64651	1.27764	-4.2753
H	6.10625	2.40638	-2.98131
H	6.40985	0.66415	-2.78555
C	-4.21641	3.00305	4.32548
H	-4.62556	4.00855	4.15077
H	-4.94444	2.276	3.92918
H	-4.14477	2.83898	5.41047

***Re*-face TS4**



Cu	0.38065	-0.55231	-0.04231
C	3.52854	-1.39344	2.52424
C	2.52477	-0.7389	3.5422
O	1.41266	-0.39829	2.69086
O	2.64439	-1.88684	1.499
B	1.4829	-1.15425	1.54584
C	-0.3318	-2.22476	0.88826
C	3.03356	0.52759	4.21313
H	3.24747	1.31777	3.48203
H	2.27479	0.90776	4.91342
H	3.95074	0.32158	4.78573
C	2.0172	-1.71817	4.59772
H	2.79153	-1.9335	5.34845
H	1.15147	-1.27447	5.11087
H	1.69688	-2.66963	4.15061
C	4.45092	-0.37328	1.8624
H	5.20822	0.00641	2.56354
H	4.96605	-0.85137	1.01643
H	3.87661	0.47696	1.4702
C	4.34001	-2.55185	3.08058
H	5.01272	-2.94134	2.30207
H	4.95832	-2.21948	3.9283
H	3.69771	-3.37606	3.41711
C	0.33576	-3.55452	0.45823

C	-0.87487	-2.29046	2.31458
H	-1.79029	-2.90455	2.32512
H	-0.15084	-2.75663	2.99673
H	-1.14269	-1.30013	2.69659
C	1.00493	-3.46617	-0.9086
H	0.25454	-3.31206	-1.69884
H	1.72737	-2.63581	-0.9477
H	1.55305	-4.39395	-1.13601
H	1.11664	-3.77454	1.20228
C	-0.67676	-4.70327	0.47867
H	-0.19685	-5.64039	0.15476
H	-1.09507	-4.87782	1.48093
H	-1.51498	-4.49886	-0.20508
N	-1.22323	-1.73135	-0.1068
P	-2.72202	-1.12849	0.13375
O	-3.07552	-0.33534	1.37463
C	-3.89392	-2.53087	-0.0084
C	-4.83775	-2.73368	1.00229
C	-3.85159	-3.41265	-1.09609
C	-5.7269	-3.8077	0.93175
H	-4.86262	-2.03704	1.84371
C	-4.74252	-4.48129	-1.17065
H	-3.11311	-3.26263	-1.8888
C	-5.68059	-4.68105	-0.15441
H	-6.46126	-3.96102	1.72659
H	-4.70538	-5.1653	-2.02211
H	-6.37866	-5.51995	-0.21188
C	-3.04404	-0.10929	-1.3512
C	-2.2237	-0.11824	-2.48302
C	-4.11795	0.78797	-1.29572
C	-2.44662	0.77938	-3.52698
H	-1.3914	-0.8196	-2.52731
C	-4.34631	1.68305	-2.33979

H	-4.75979	0.80399	-0.41173
C	-3.50303	1.68825	-3.45269
H	-1.78961	0.77173	-4.40039
H	-5.17879	2.38841	-2.28051
H	-3.67381	2.39855	-4.26546
C	0.87977	1.01722	-1.04683
N	0.23587	2.20905	-1.05832
N	1.83065	1.19317	-1.98048
C	-0.89716	2.60929	-0.23959
C	0.81372	3.02274	-1.99026
N	1.80767	2.42424	-2.57138
C	2.8774	0.26574	-2.28094
C	-0.78703	2.25676	1.25013
C	-1.0698	4.16889	-0.22924
H	-1.78652	2.13669	-0.67375
C	0.29486	4.41521	-2.13459
C	4.15208	0.51048	-1.75293
C	2.59234	-0.85804	-3.06601
C	0.53806	2.81199	1.79568
H	-0.97286	1.19285	1.45173
C	-1.84494	3.22756	1.84651
C	-1.13715	4.50335	1.28028
H	-2.01523	4.43187	-0.73487
O	-0.0259	4.88258	-0.85285
H	-0.58553	4.42684	-2.80597
H	1.06555	5.06701	-2.56403
C	5.14904	-0.43618	-1.99962
C	4.44155	1.76158	-0.97127
C	3.61973	-1.7794	-3.27888
C	1.22092	-1.07249	-3.63847
H	0.74399	2.38998	2.78737
H	1.39374	2.53255	1.16504
C	0.29533	4.34178	1.83435

C	-3.2737	2.99837	1.33498
C	-1.91244	3.16569	3.37519
C	-1.78017	5.84657	1.56416
C	4.89876	-1.59228	-2.74547
H	6.14839	-0.26768	-1.58835
H	4.49822	2.6326	-1.64314
H	3.65005	1.97483	-0.23728
H	5.39711	1.67887	-0.43672
H	3.41177	-2.6704	-3.87803
H	0.51605	-1.35296	-2.84254
H	0.83534	-0.15707	-4.11174
H	1.22588	-1.8784	-4.384
H	0.34706	4.73895	2.85853
H	1.01683	4.90527	1.22983
H	-3.54221	1.94251	1.49226
H	-3.98214	3.63401	1.88894
H	-3.41533	3.21826	0.26797
H	-2.57041	3.95914	3.76339
H	-2.34387	2.20086	3.68425
H	-0.94052	3.26641	3.8751
H	-1.82961	6.04245	2.6465
H	-1.20116	6.66168	1.10225
H	-2.80463	5.89402	1.16156
C	5.9722	-2.62754	-2.94714
H	5.87728	-3.12013	-3.9257
H	6.97664	-2.18667	-2.87411
H	5.89813	-3.41213	-2.17609

10. Reference

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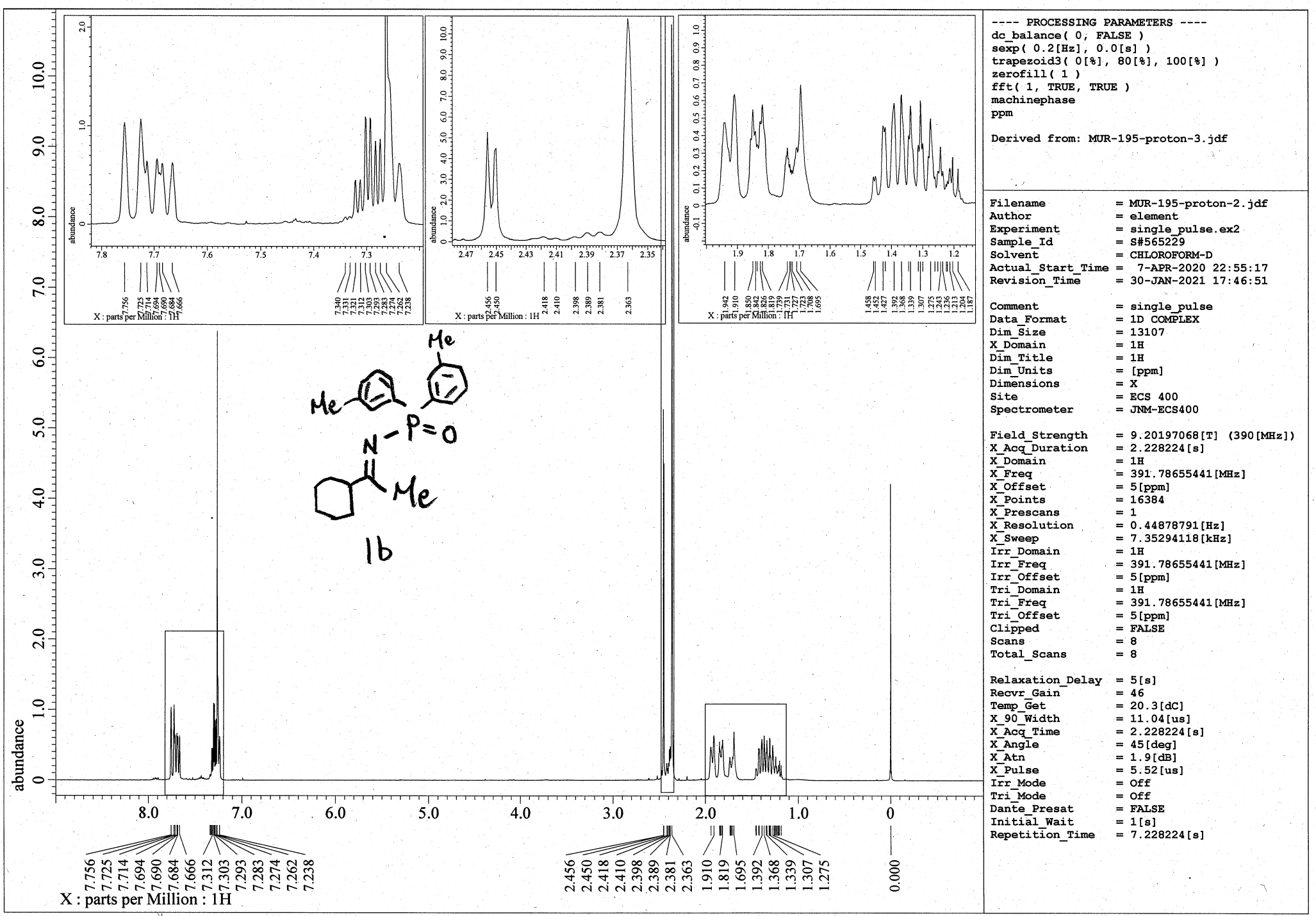
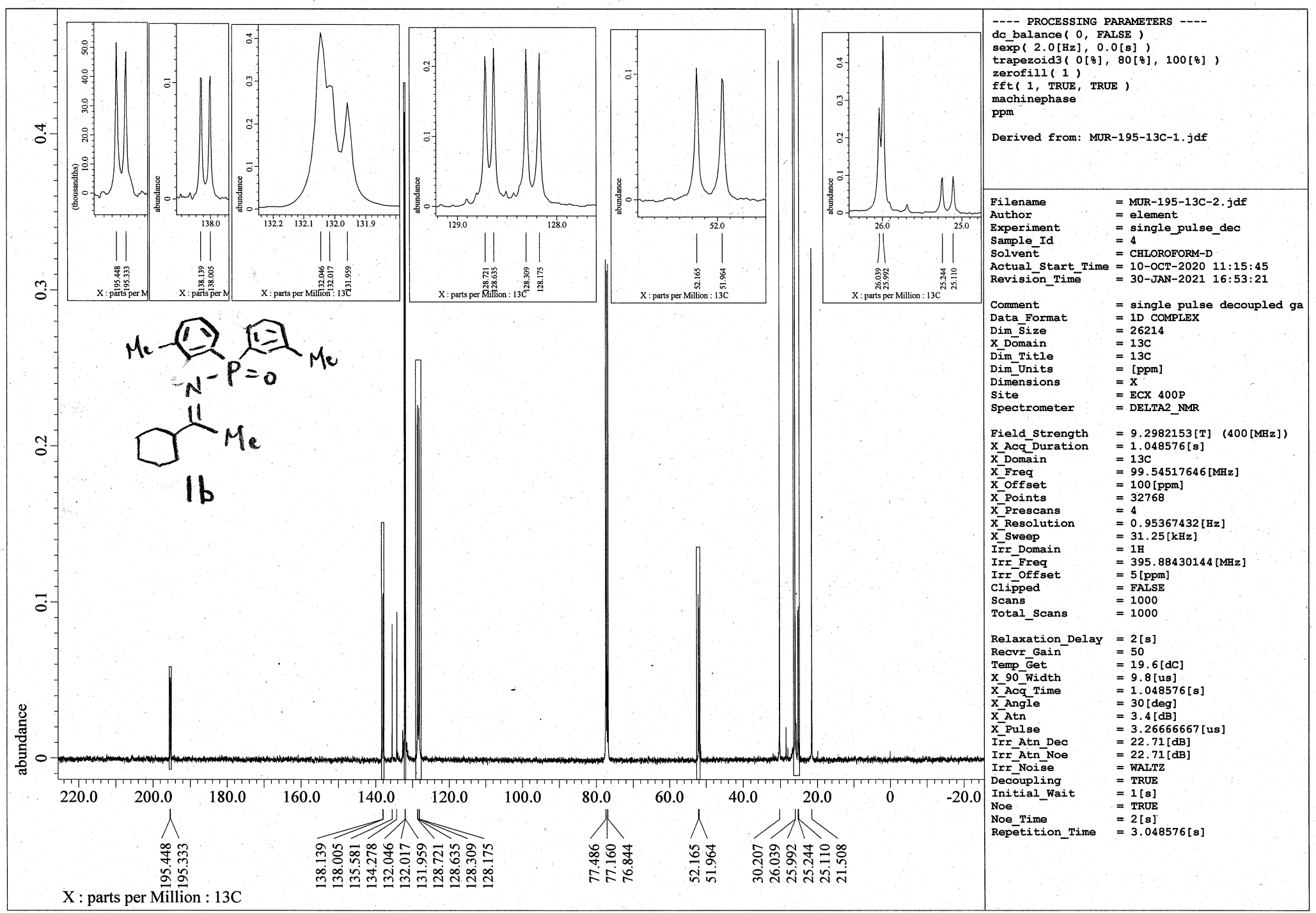


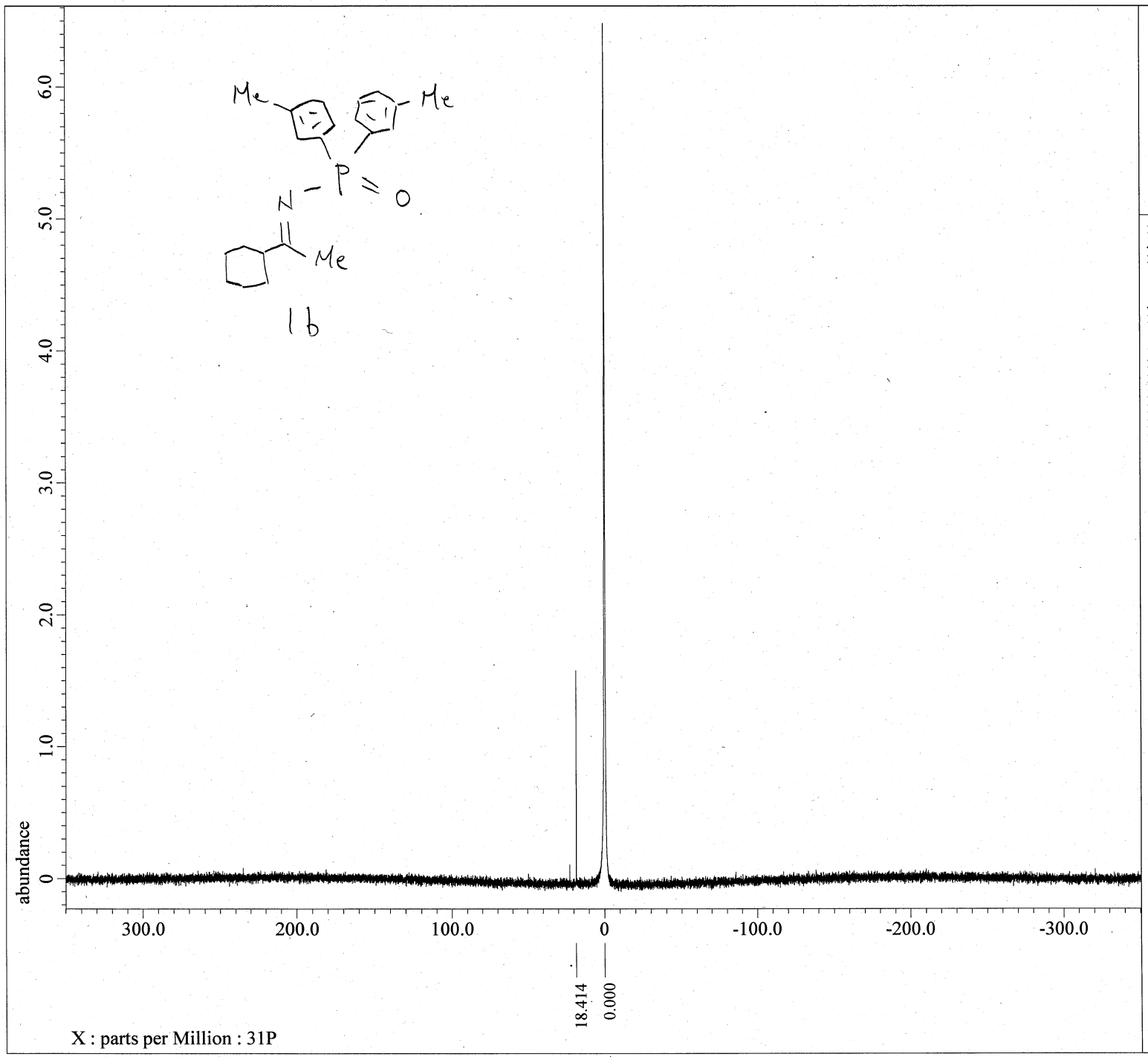

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-195-proton-3.jdf
```

```
Filename            = MUR-195-proton-2.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#565229
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-APR-2020 22:55:17
Revision_Time       = 30-JAN-2021 17:46:51

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          = 46
Temp_Get            = 20.3[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]
```




```
---- 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: MUR-195-13C-1.jdf
```

Filename	= MUR-195-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 4
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-OCT-2020 11:15:45
Revision_Time	= 30-JAN-2021 16:53:21
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 1.048576[s]
X_Domain	= 13C
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1000
Total_Scans	= 1000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.6[dC]
X_90_Width	= 9.8[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 3.26666667[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Atn_Noe	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.048576[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

Derived from: MUR-195-31P-1.jdf
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Filename            = MUR-195-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#403338
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-APR-2021 17:57:59
Revision_Time       =  6-MAY-2021 19:23:33

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 48
Temp_Get            = 18.9[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
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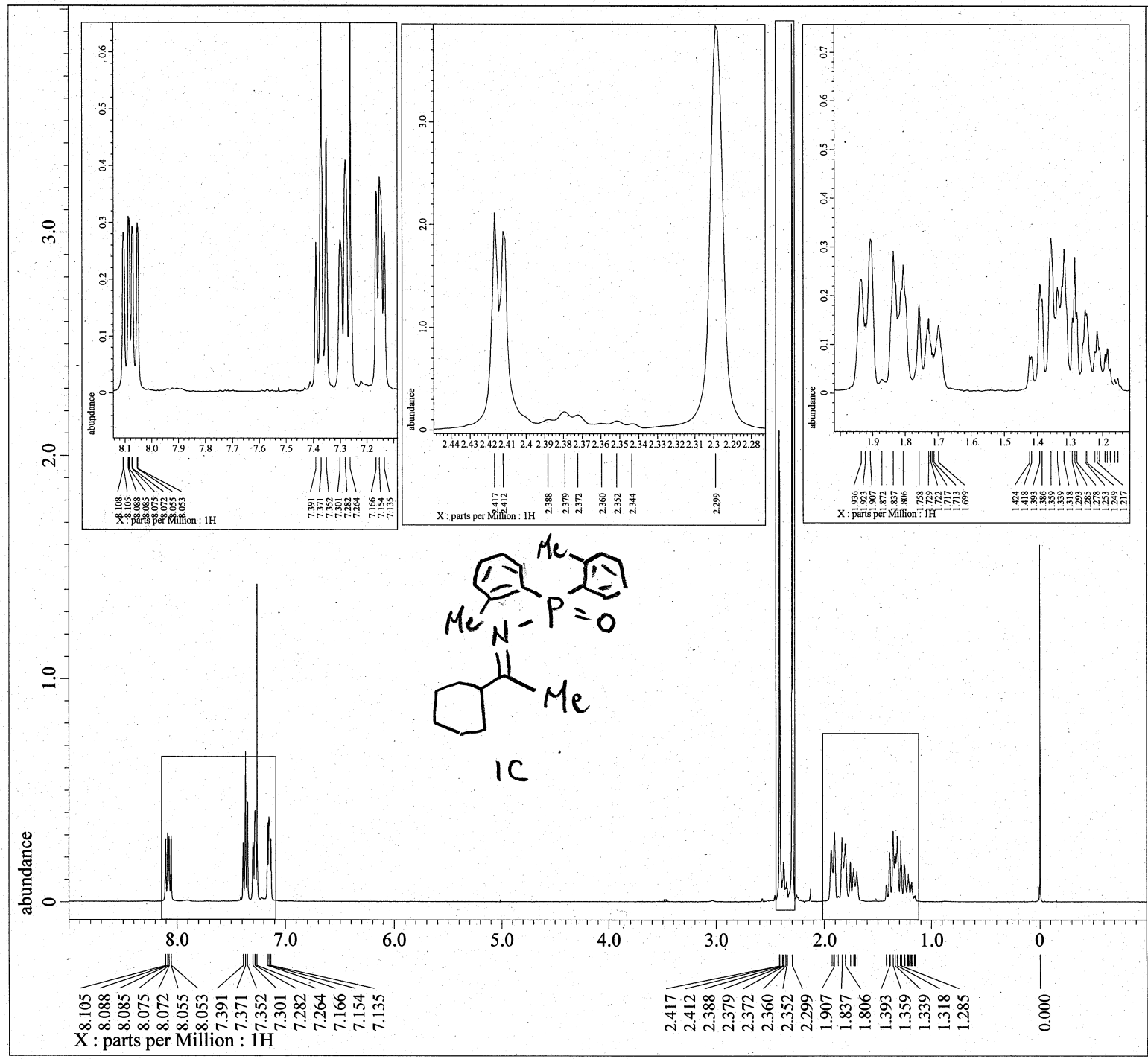


```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-cy-me-ketimine-otol-1.jdf
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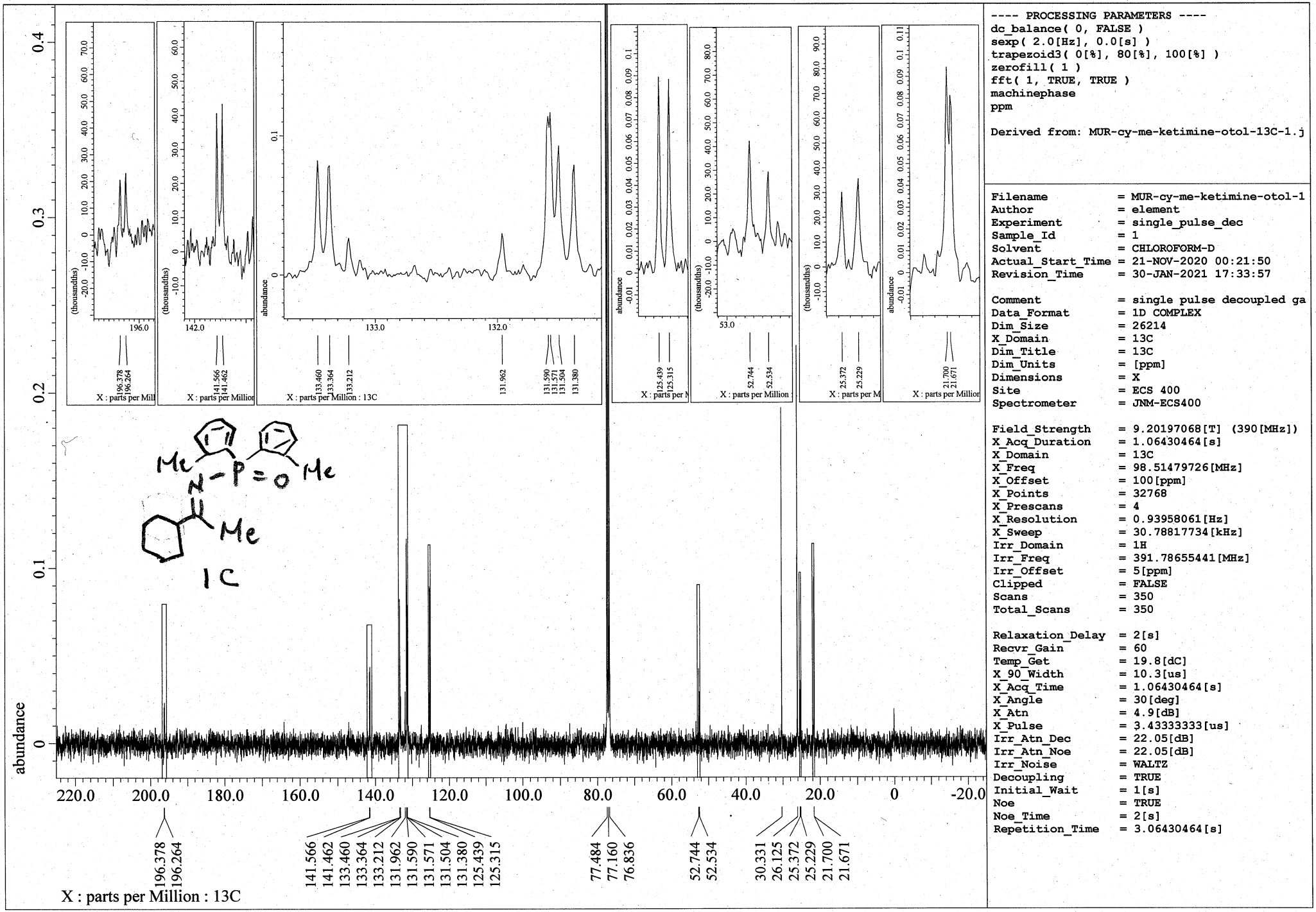
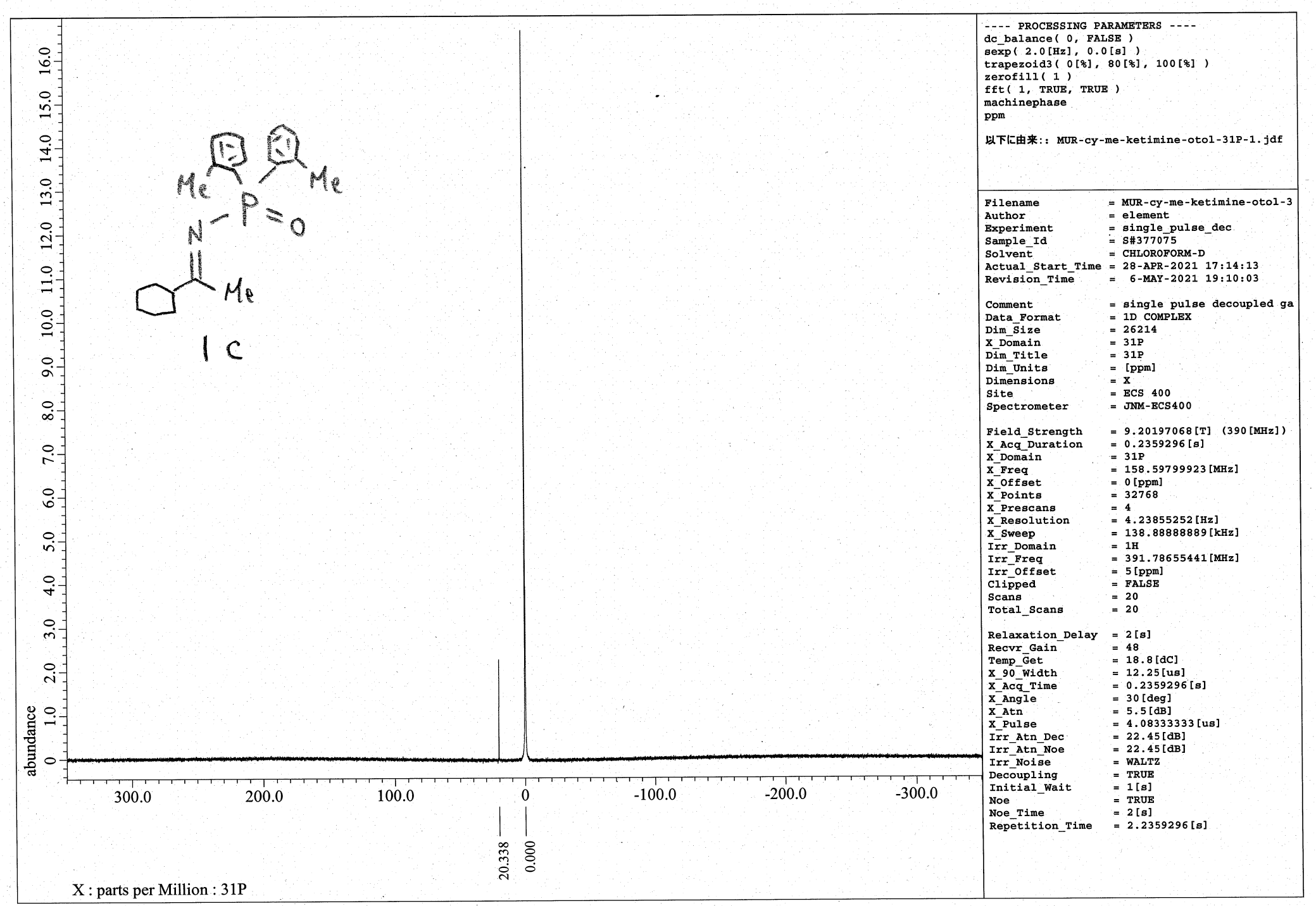
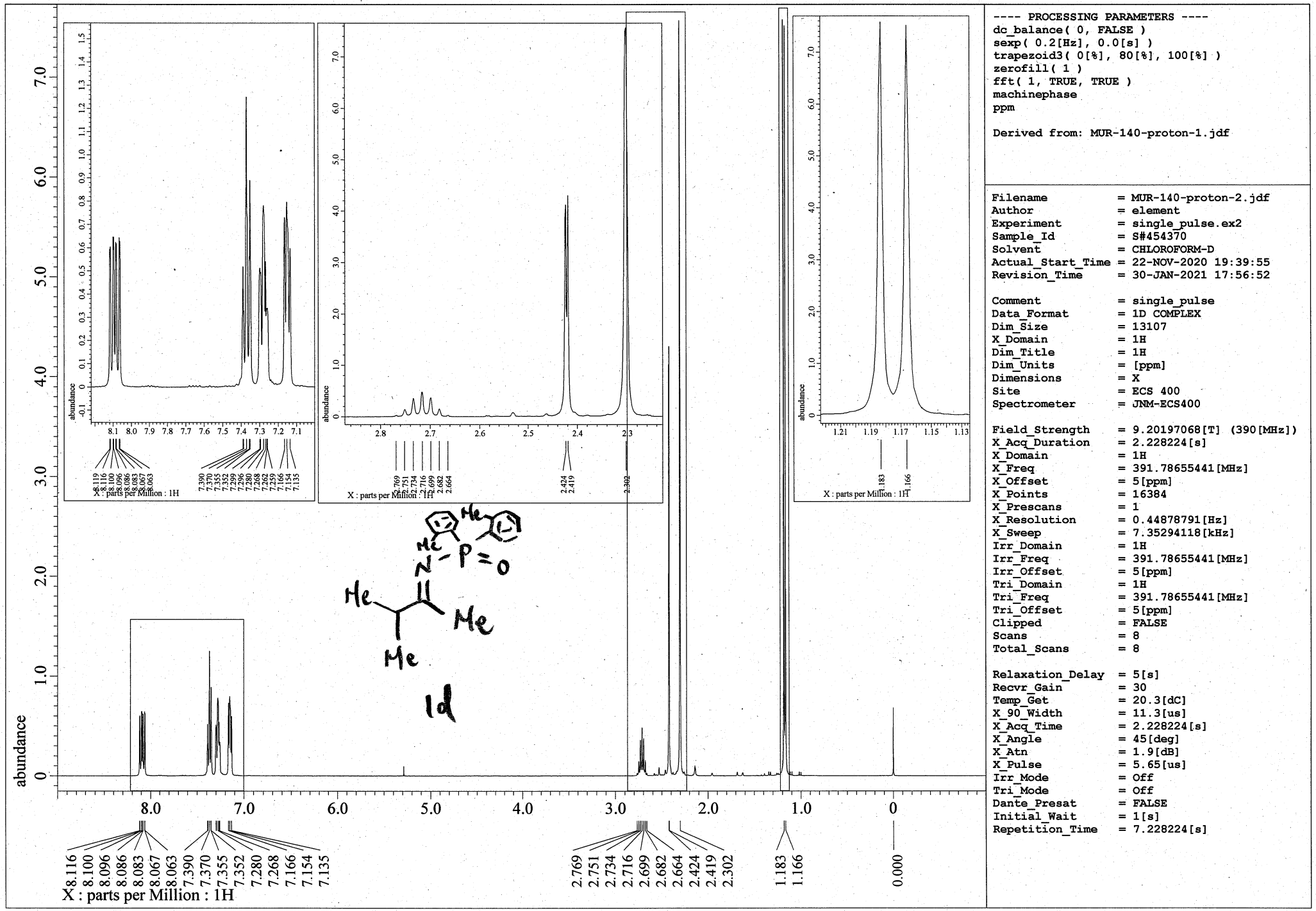
Filename	= MUR-cy-me-ketimine-otol-2
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#620412
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-NOV-2020 00:17:10
Revision_Time	= 30-JAN-2021 17:16:09
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [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	= 36
Temp_Get	= 19.4[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]

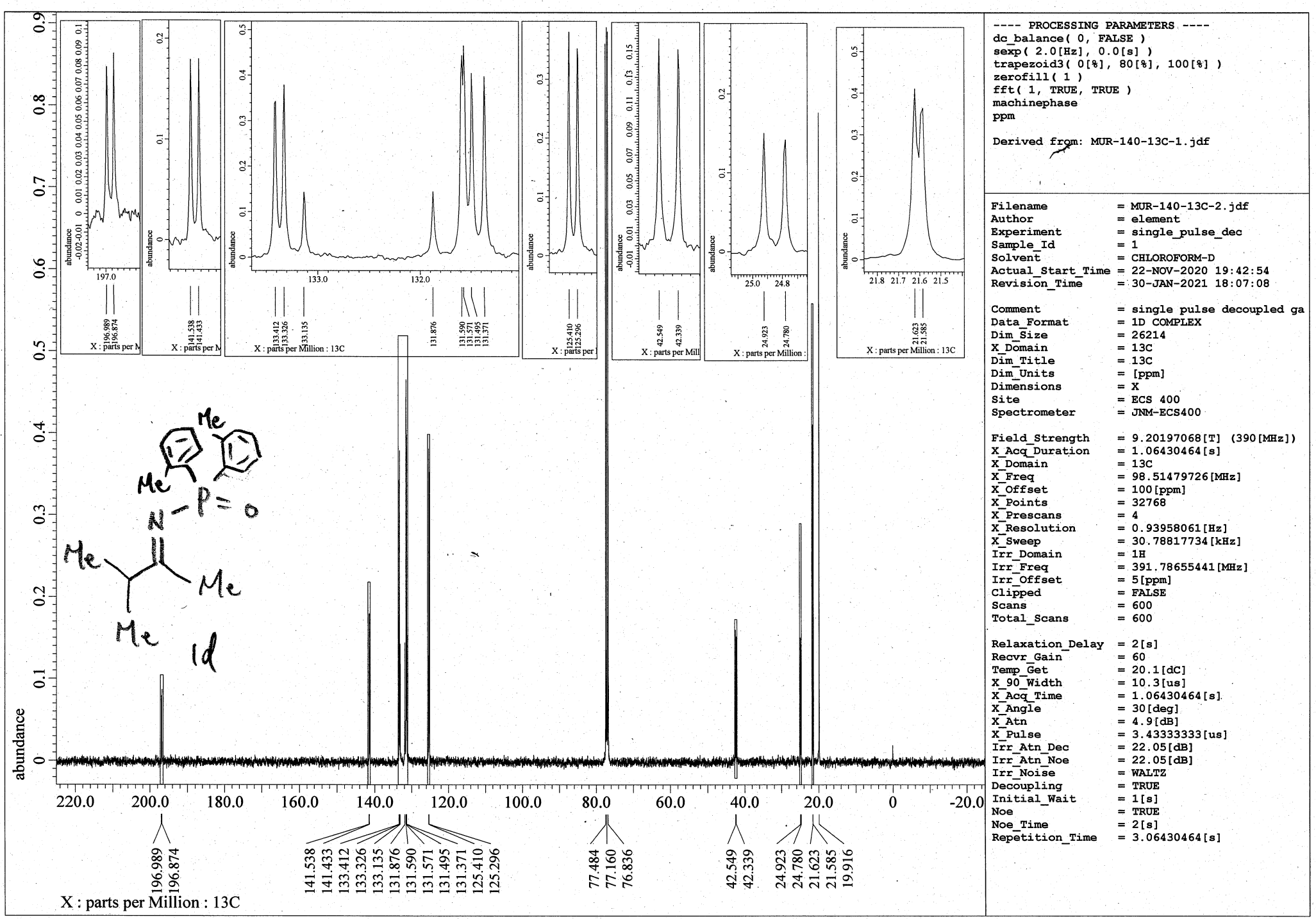

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-cy-me-ketimine-otol-13C-1.j
Filename = MUR-cy-me-ketimine-otol-1
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-NOV-2020 00:21:50
Revision_Time = 30-JAN-2021 17:33:57
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 350
Total_Scans = 350
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.8[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.43333333[us]
Irr_Atn_Dec = 22.05[dB]
Irr_Atn_Noe = 22.05[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
Me
N
P
O
Me
Me
1C
abundance
220.0
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0
-20.0
196.378
196.264
141.566
141.462
133.460
133.364
133.212
131.962
131.590
131.571
131.504
131.380
125.439
125.315
77.484
77.160
76.836
52.744
52.534
30.331
26.125
25.372
25.229
21.700
21.671
X : parts per Million : 13C




```
---- 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:: MUR-cy-me-ketimine-otol-31P-1.jdf
```

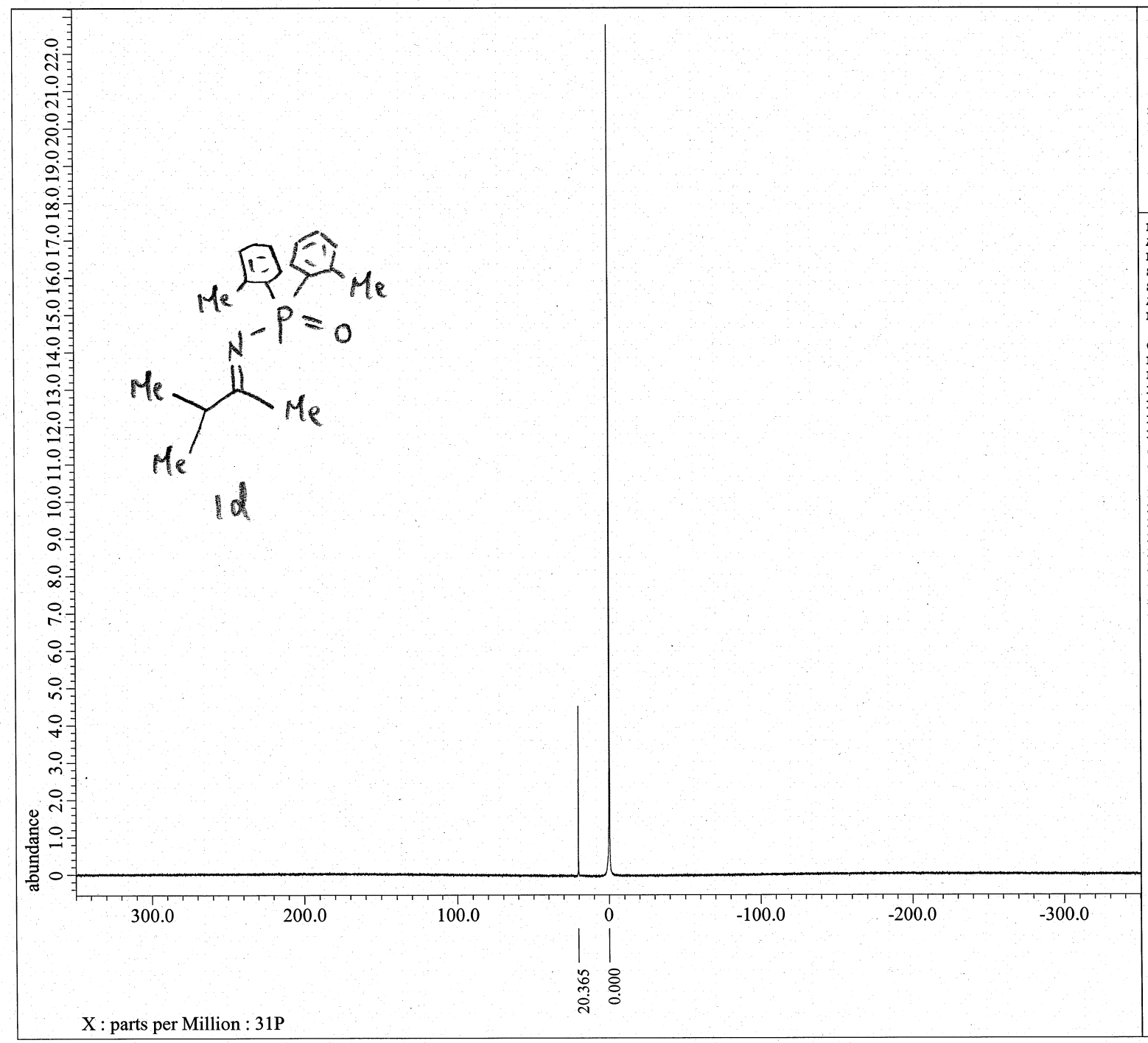
Filename	= MUR-cy-me-ketimine-otol-3
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#377075
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-APR-2021 17:14:13
Revision_Time	= 6-MAY-2021 19:10:03
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 31P
Dim_Title	= 31P
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 0.2359296[s]
X_Domain	= 31P
X_Freq	= 158.59799923[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 4.23855252[Hz]
X_Sweep	= 138.88888889[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 20
Total_Scans	= 20
Relaxation_Delay	= 2[s]
Recvr_Gain	= 48
Temp_Get	= 18.8[dC]
X_90_Width	= 12.25[us]
X_Acq_Time	= 0.2359296[s]
X_Angle	= 30[deg]
X_Atn	= 5.5[dB]
X_Pulse	= 4.08333333[us]
Irr_Atn_Dec	= 22.45[dB]
Irr_Atn_Noe	= 22.45[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.2359296[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
Derived from: MUR-140-proton-1.jdf
Filename = MUR-140-proton-2.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#454370
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-NOV-2020 19:39:55
Revision_Time = 30-JAN-2021 17:56:52
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 = 30
Temp_Get = 20.3[dC]
X_90_Width = 11.3[us]
X_Acq_Time = 2.228224[s]
X_Angle = 45[deg]
X_Atn = 1.9[dB]
X_Pulse = 5.65[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.228224[s]
abundance
X : parts per Million : 1H
8.116 8.100 8.096 8.086 8.083 8.067 8.063 7.390 7.370 7.355 7.352 7.280 7.268 7.166 7.154 7.135
2.769 2.751 2.734 2.716 2.699 2.682 2.664 2.424 2.419 2.302
1.183 1.166
0.000
Me
Me
Me
N
P
O
Me
Me
1d



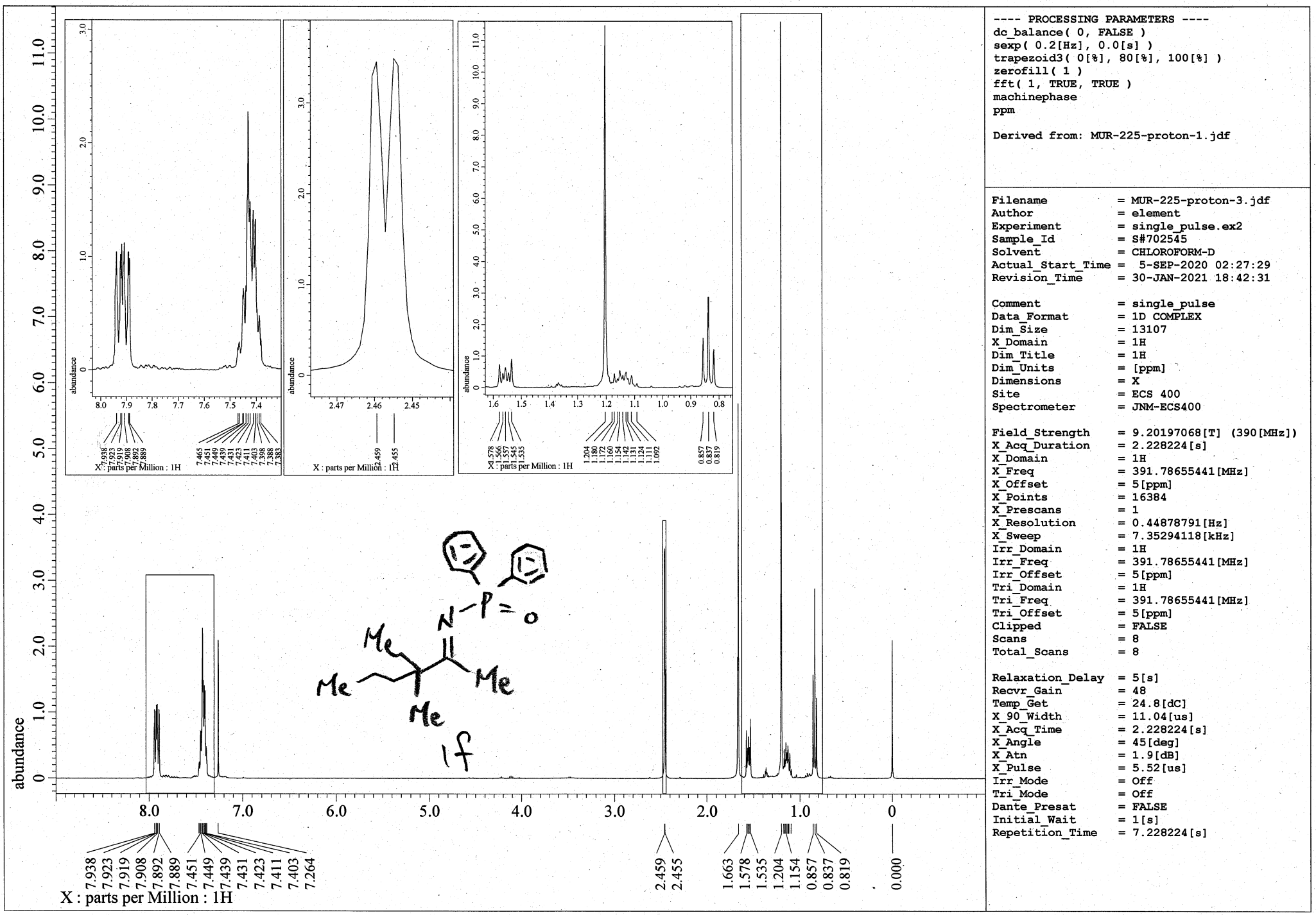

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-140-13C-1.jdf
```

Filename	= MUR-140-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-NOV-2020 19:42:54
Revision_Time	= 30-JAN-2021 18:07:08
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 600
Total_Scans	= 600
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.1[dC]
X_90_Width	= 10.3[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.43333333[us]
Irr_Atn_Dec	= 22.05[dB]
Irr_Atn_Noe	= 22.05[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[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:: MUR-140-31P-1.jdf
```

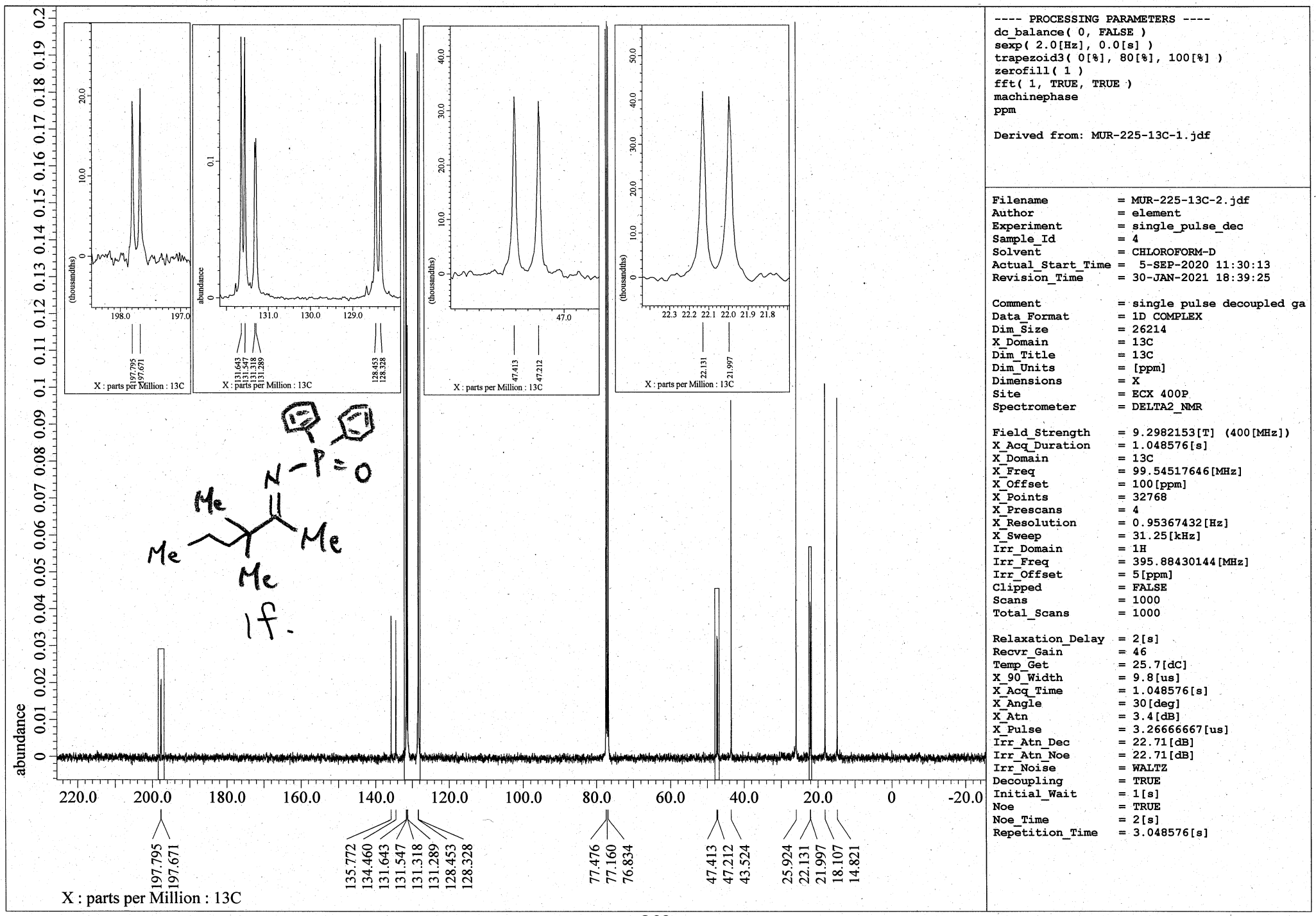
Filename	= MUR-140-31P-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#382737
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-APR-2021 17:23:42
Revision_Time	= 6-MAY-2021 19:11:14
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 31P
Dim_Title	= 31P
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 0.2359296[s]
X_Domain	= 31P
X_Freq	= 158.59799923[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 4.23855252[Hz]
X_Sweep	= 138.88888889[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 20
Total_Scans	= 20
Relaxation_Delay	= 2[s]
Recvr_Gain	= 46
Temp_Get	= 18.8[dC]
X_90_Width	= 12.25[us]
X_Acq_Time	= 0.2359296[s]
X_Angle	= 30[deg]
X_Atn	= 5.5[dB]
X_Pulse	= 4.08333333[us]
Irr_Atn_Dec	= 22.45[dB]
Irr_Atn_Noe	= 22.45[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.2359296[s]

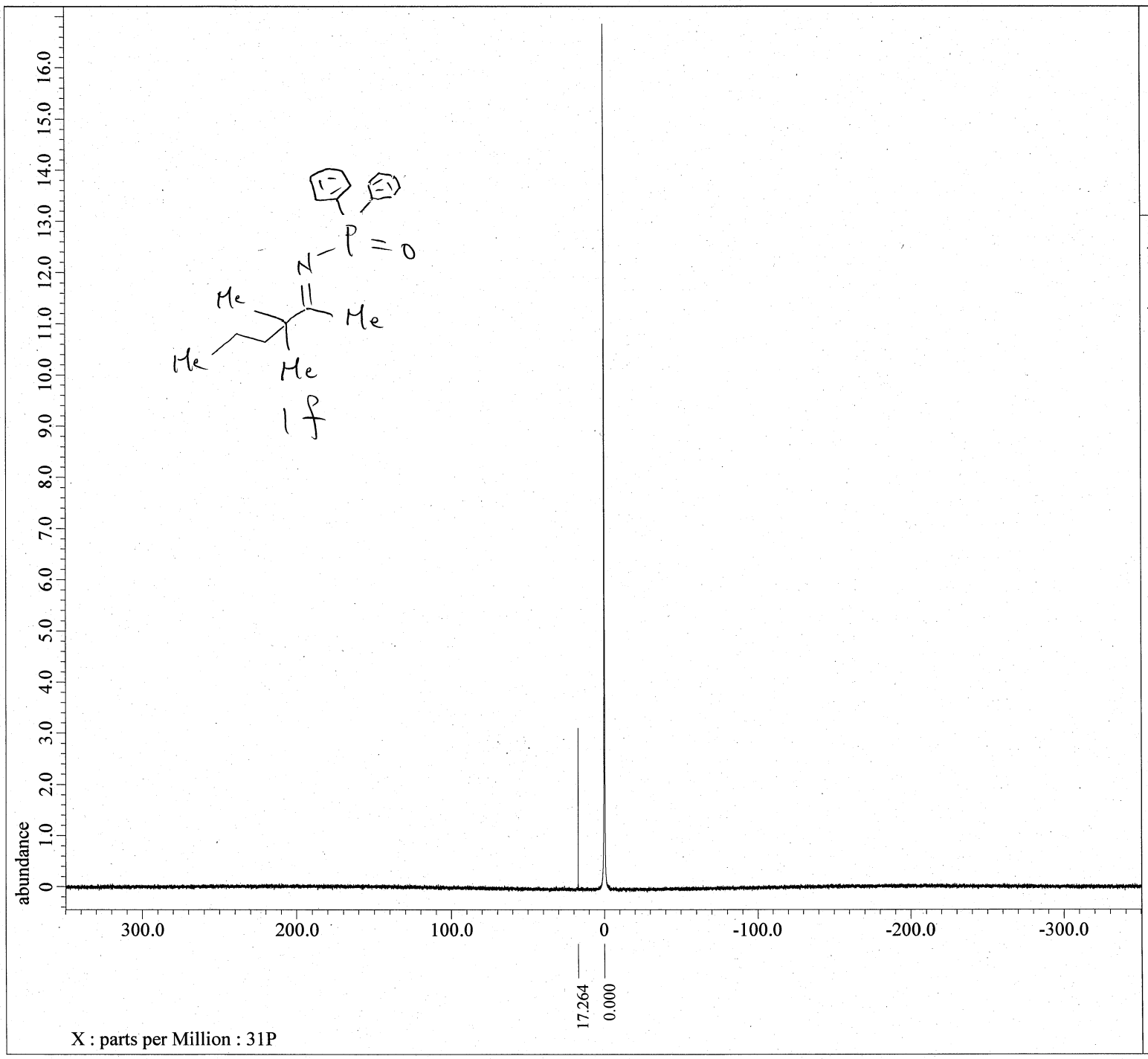


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm

Derived from: MUR-225-proton-1.jdf

Filename	= MUR-225-proton-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#702545
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-SEP-2020 02:27:29
Revision_Time	= 30-JAN-2021 18:42:31
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	= 48
Temp_Get	= 24.8[dC]
X_90_Width	= 11.04[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.52[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]

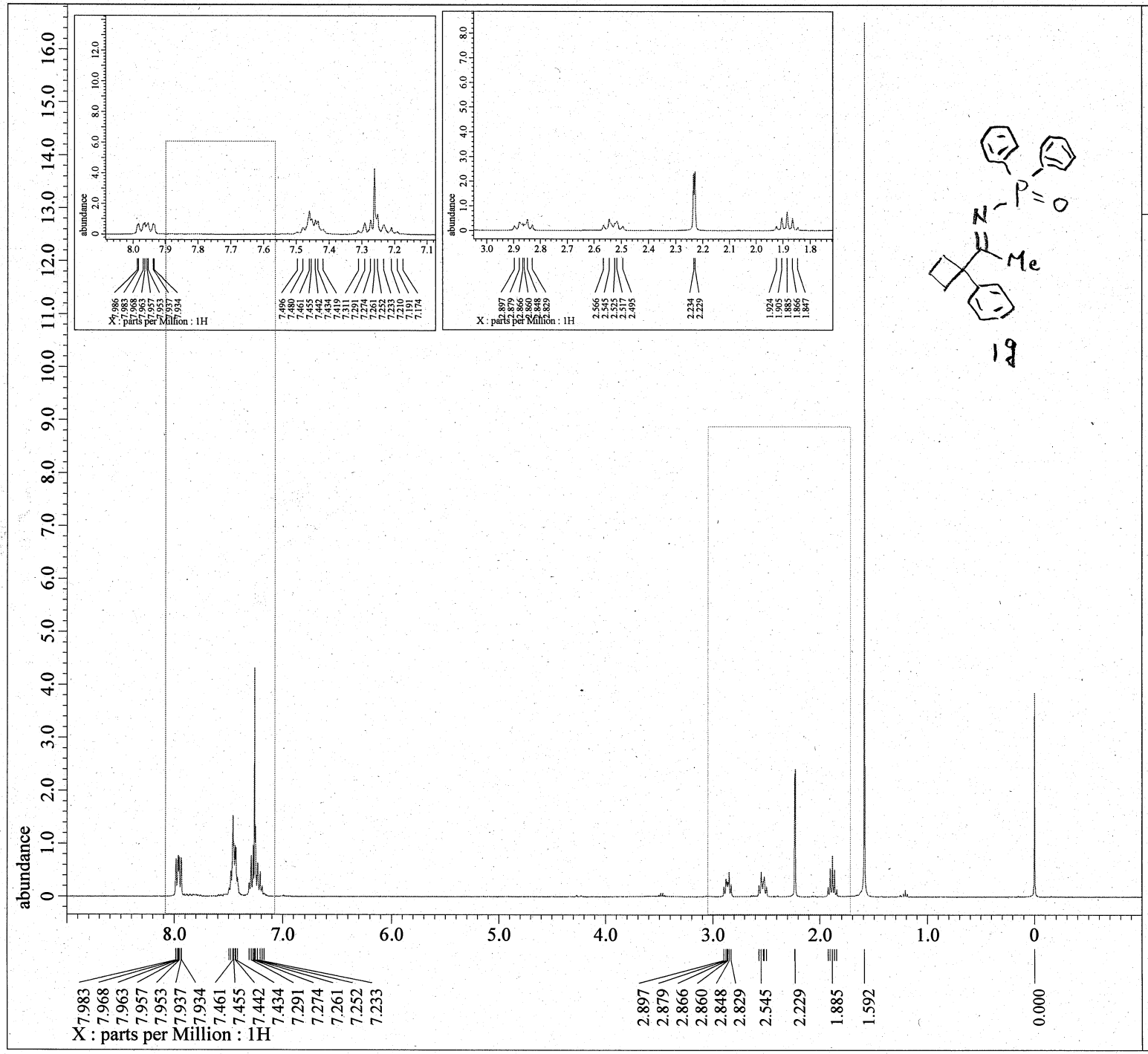

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-225-13C-1.jdf
Filename = MUR-225-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 4
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2020 11:30:13
Revision_Time = 30-JAN-2021 18:39:25
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 46
Temp_Get = 25.7[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[s]
abundance
X : parts per Million : 13C
197.795
197.671
135.772
134.460
131.643
131.547
131.318
131.289
128.453
128.328
77.476
77.160
76.834
47.413
47.212
43.524
25.924
22.131
21.997
18.107
14.821
Me
Me
Me
Me
N
P
O
1f.



1f

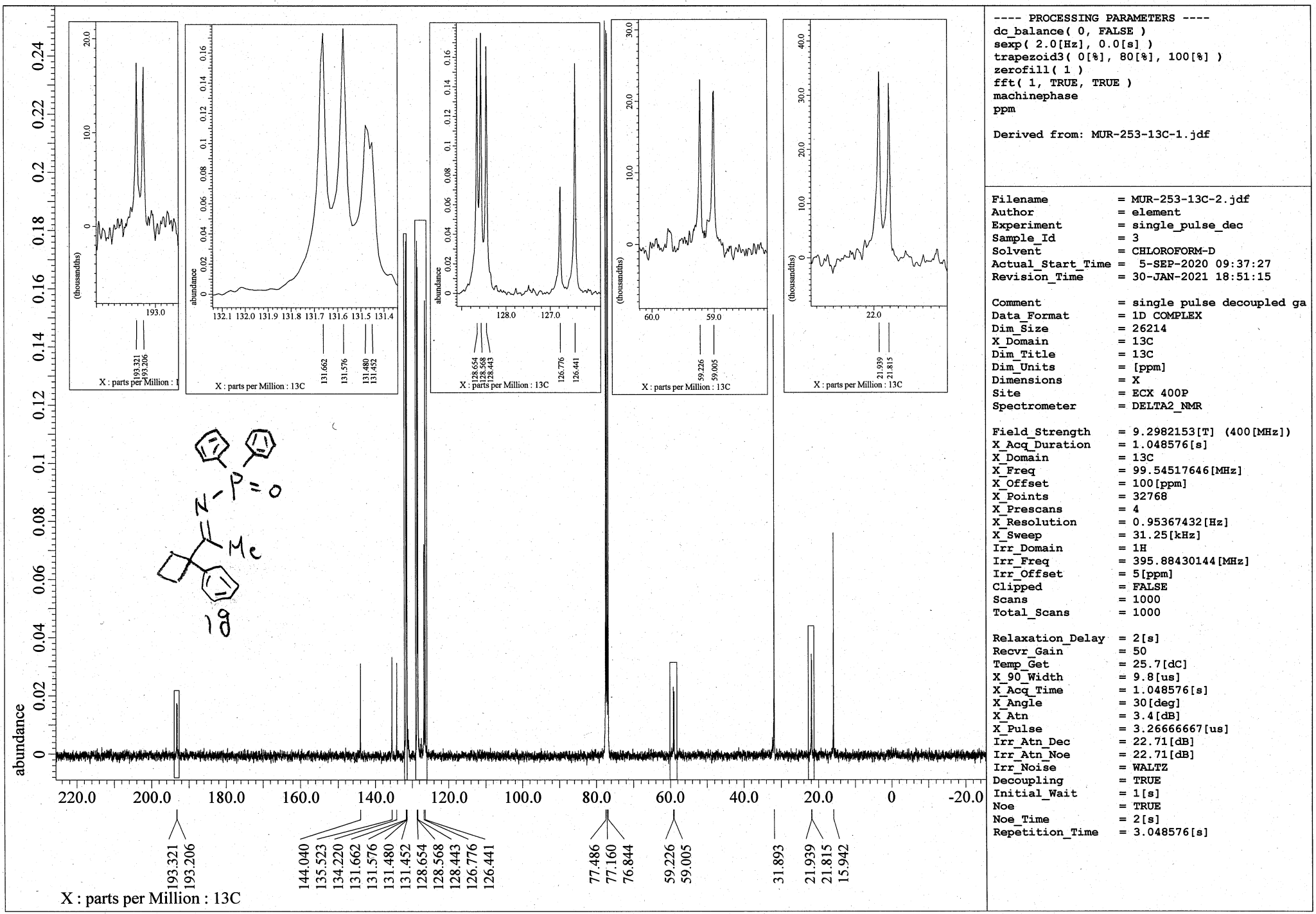
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-225-31P-1.jdf
```

```
Filename            = MUR-225-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#440251
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-APR-2021 18:59:30
Revision_Time       =  6-MAY-2021 19:24:08

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 48
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```



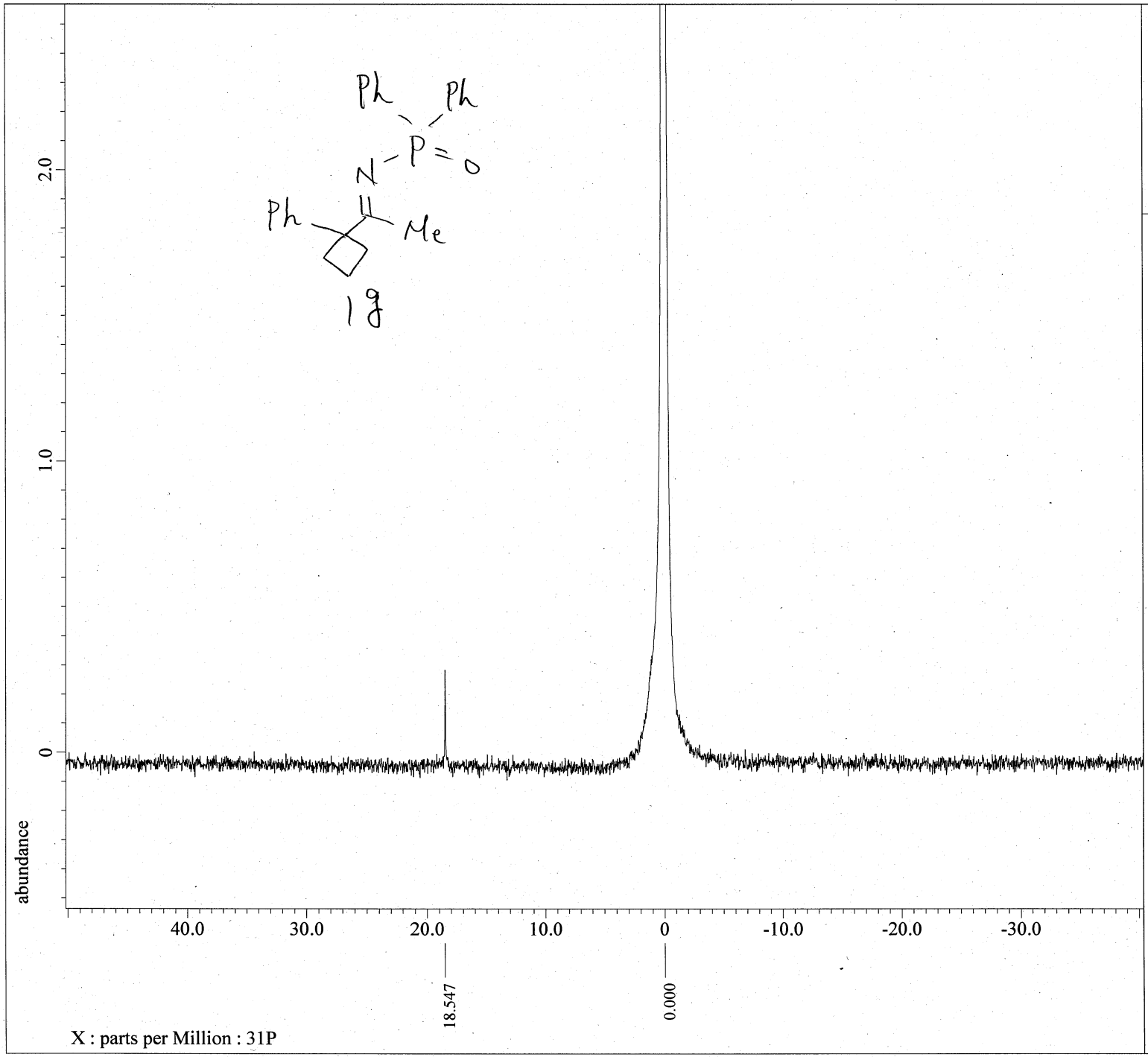

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-253-proton-1.jdf
```

Filename	= MUR-253-proton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#693671
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-SEP-2020 02:12:44
Revision_Time	= 24-OCT-2020 15:02:22
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	= 24.9[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]



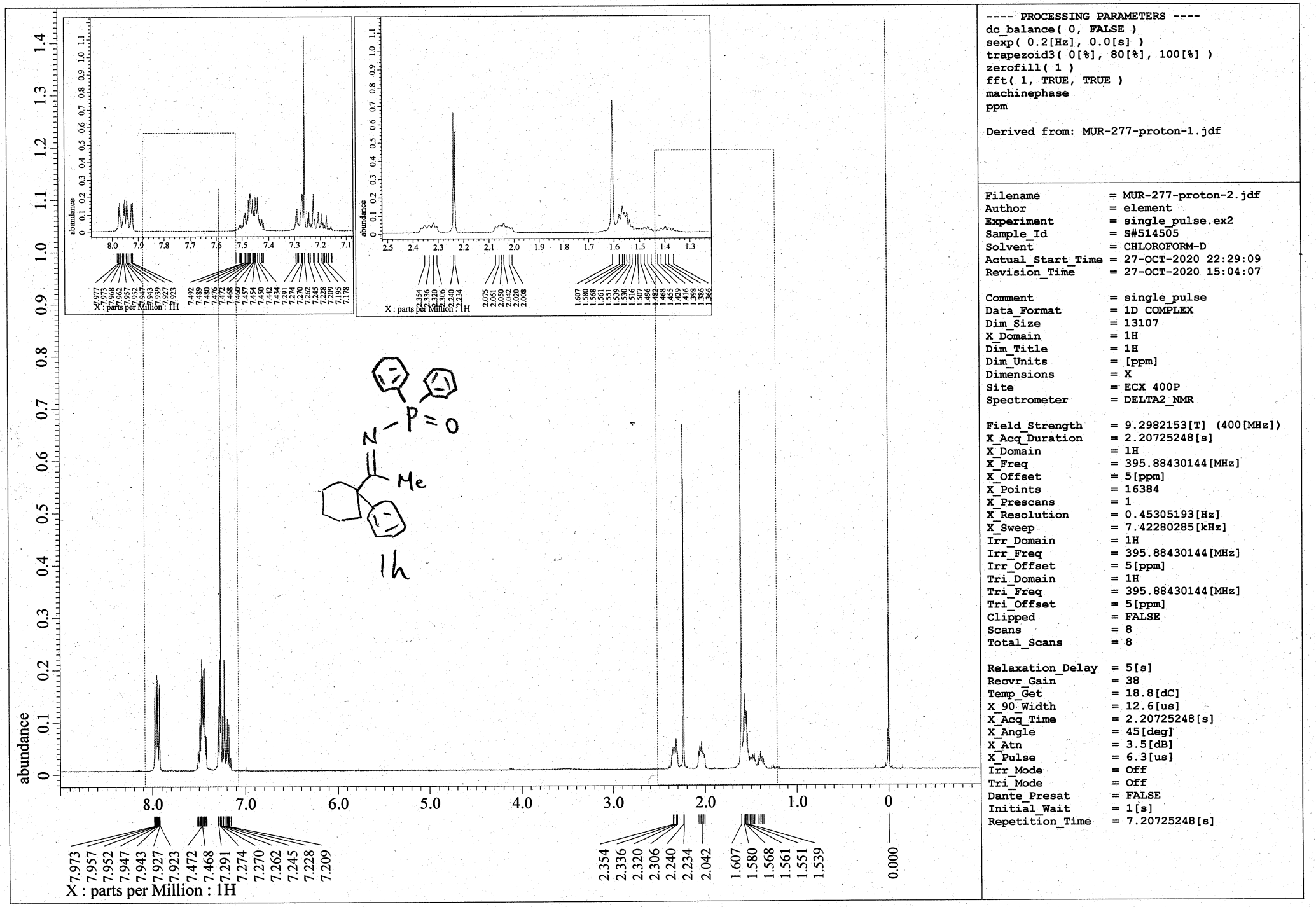

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-253-13C-1.jdf
```

Filename	= MUR-253-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-SEP-2020 09:37:27
Revision_Time	= 30-JAN-2021 18:51:15
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 1.048576[s]
X_Domain	= 13C
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1000
Total_Scans	= 1000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 25.7[dC]
X_90_Width	= 9.8[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 3.26666667[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Atn_Noe	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.048576[s]



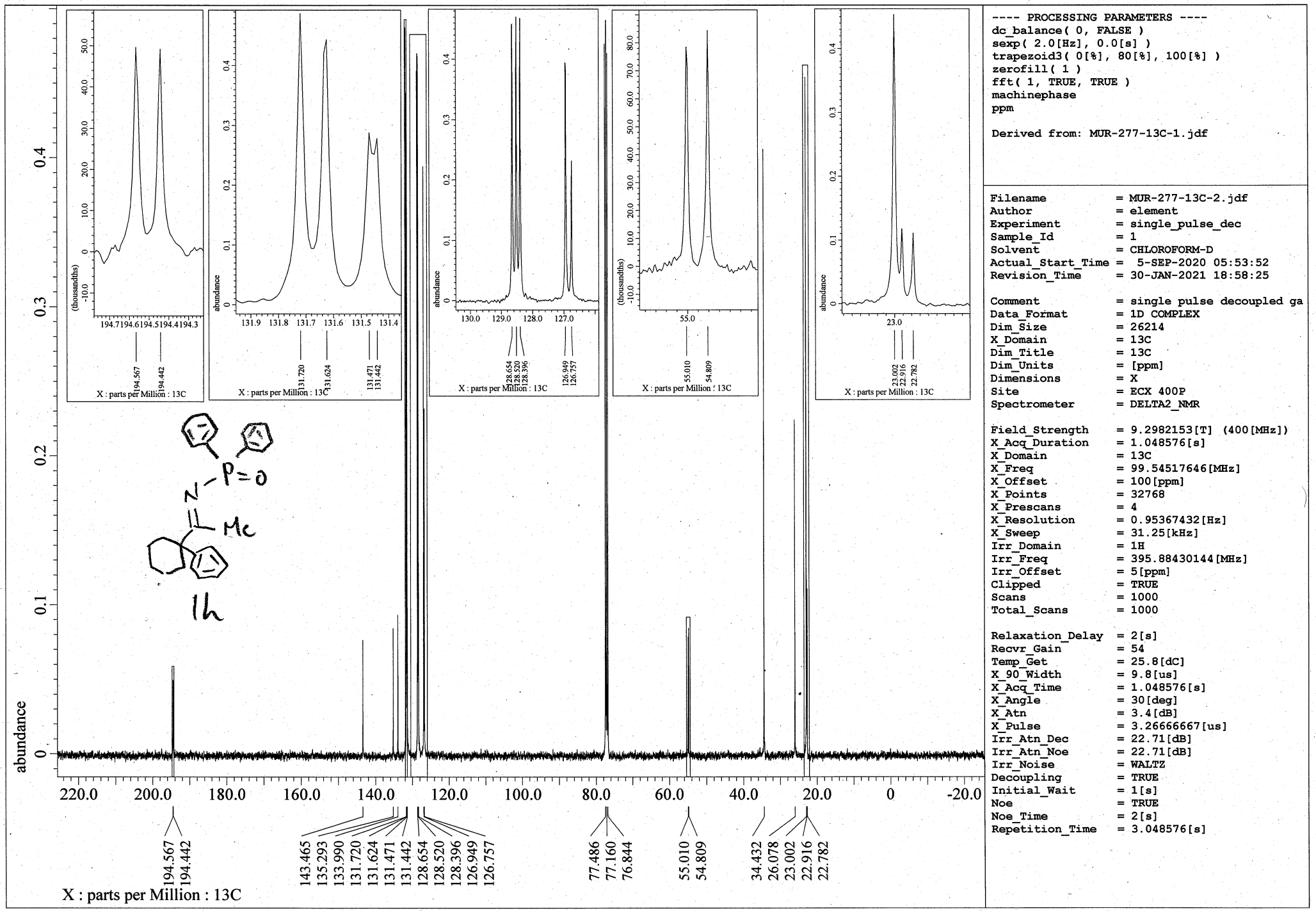

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-253-31P-1.jdf
```

```
Filename            = MUR-253-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#446872
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-APR-2021 19:10:32
Revision_Time       =  6-MAY-2021 19:26:01

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 46
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```



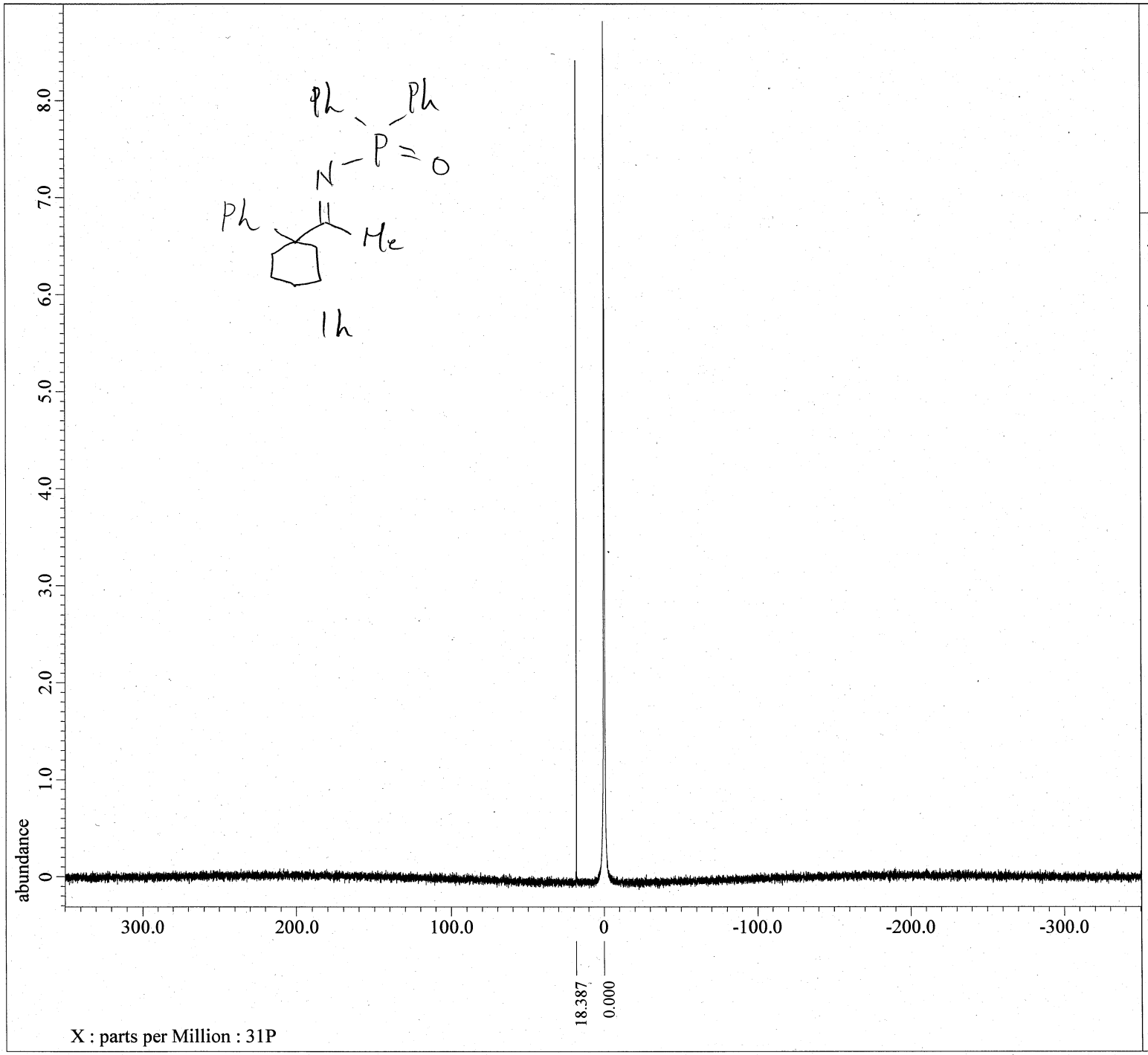

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-277-proton-1.jdf
```

Filename	= MUR-277-proton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#514505
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-OCT-2020 22:29:09
Revision_Time	= 27-OCT-2020 15:04:07
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 2.20725248[s]
X_Domain	= 1H
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 38
Temp_Get	= 18.8[dC]
X_90_Width	= 12.6[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 6.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.20725248[s]



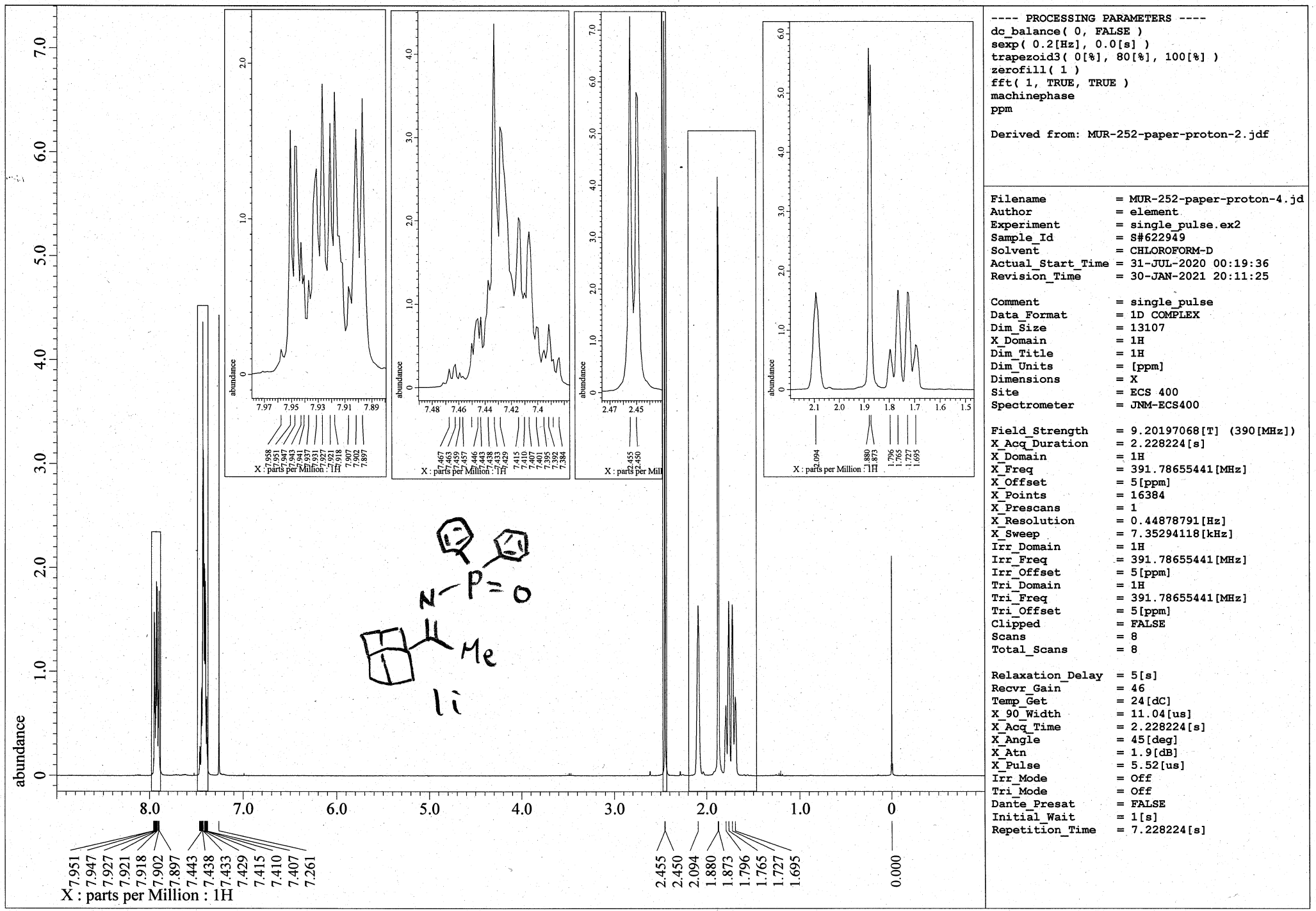

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-277-13C-1.jdf
```

Filename	= MUR-277-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-SEP-2020 05:53:52
Revision_Time	= 30-JAN-2021 18:58:25
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 1.048576[s]
X_Domain	= 13C
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= TRUE
Scans	= 1000
Total_Scans	= 1000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 54
Temp_Get	= 25.8[dC]
X_90_Width	= 9.8[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 3.26666667[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Atn_Noe	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.048576[s]



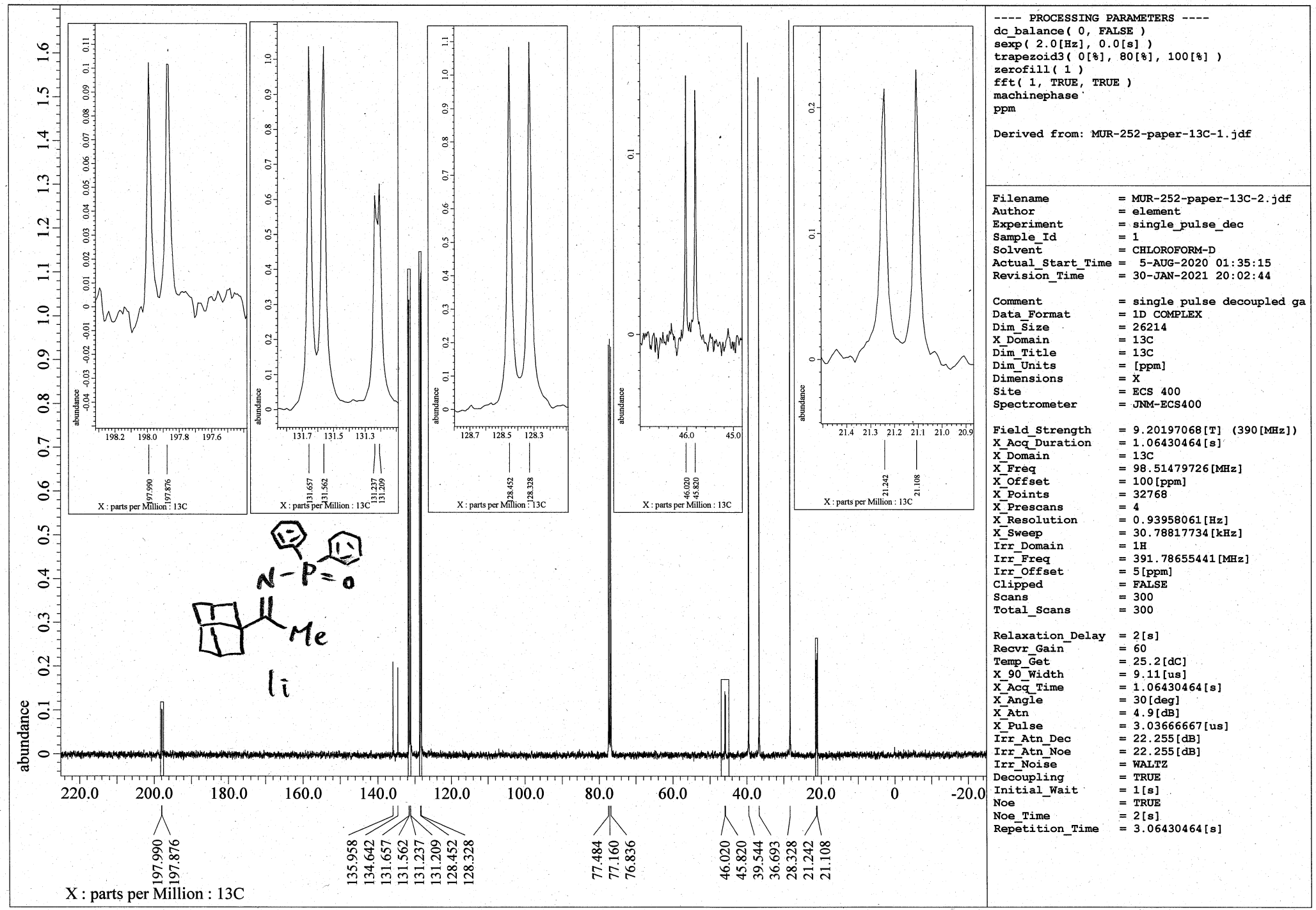

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-277-31P-1.jdf
```

```
Filename            = MUR-277-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#472047
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-APR-2021 19:52:25
Revision_Time       =  6-MAY-2021 19:27:40

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```



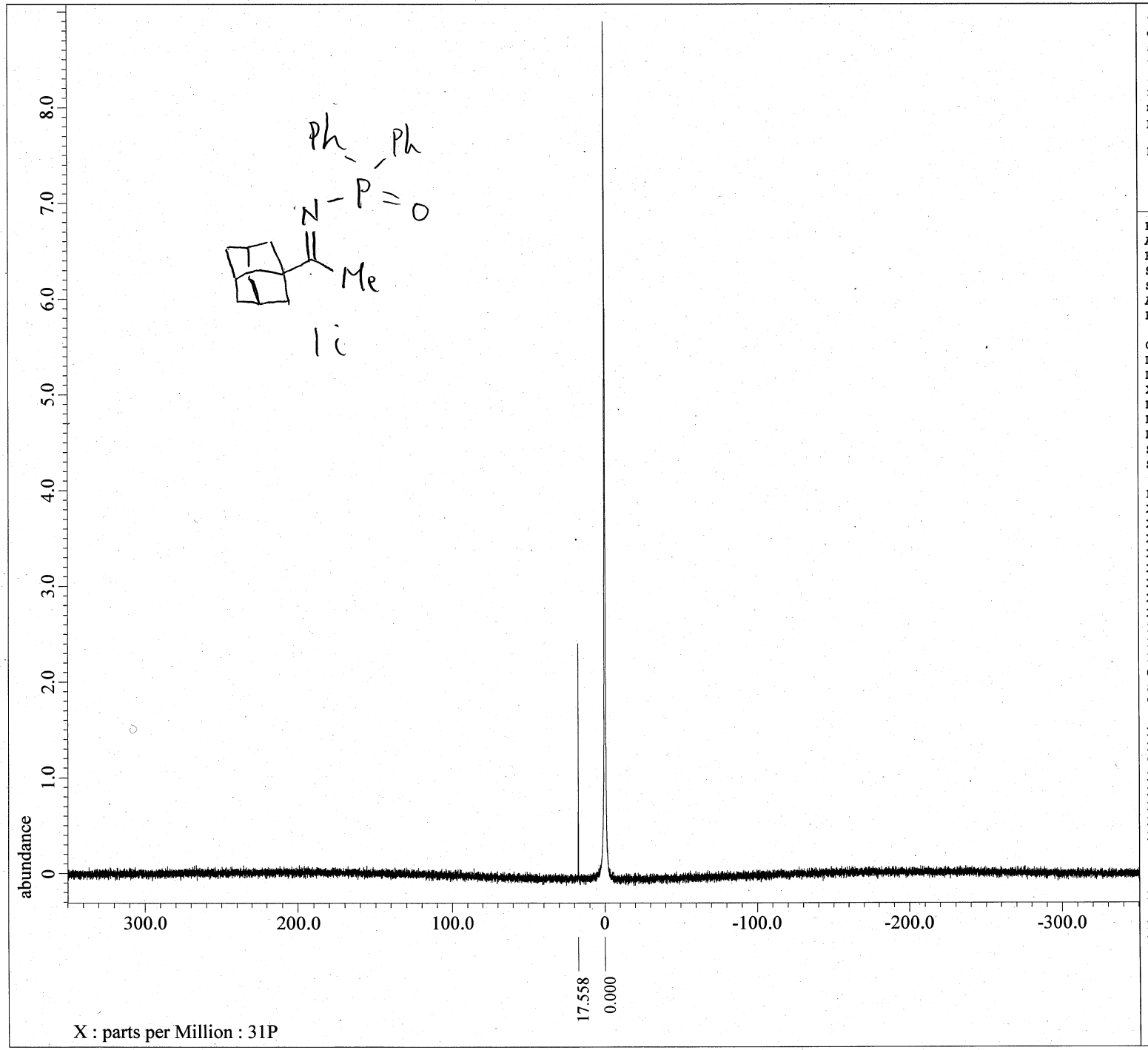

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-252-paper-proton-2.jdf
```

Filename	= MUR-252-paper-proton-4.jd
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#622949
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-JUL-2020 00:19:36
Revision_Time	= 30-JAN-2021 20:11:25
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	= 46
Temp_Get	= 24[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]



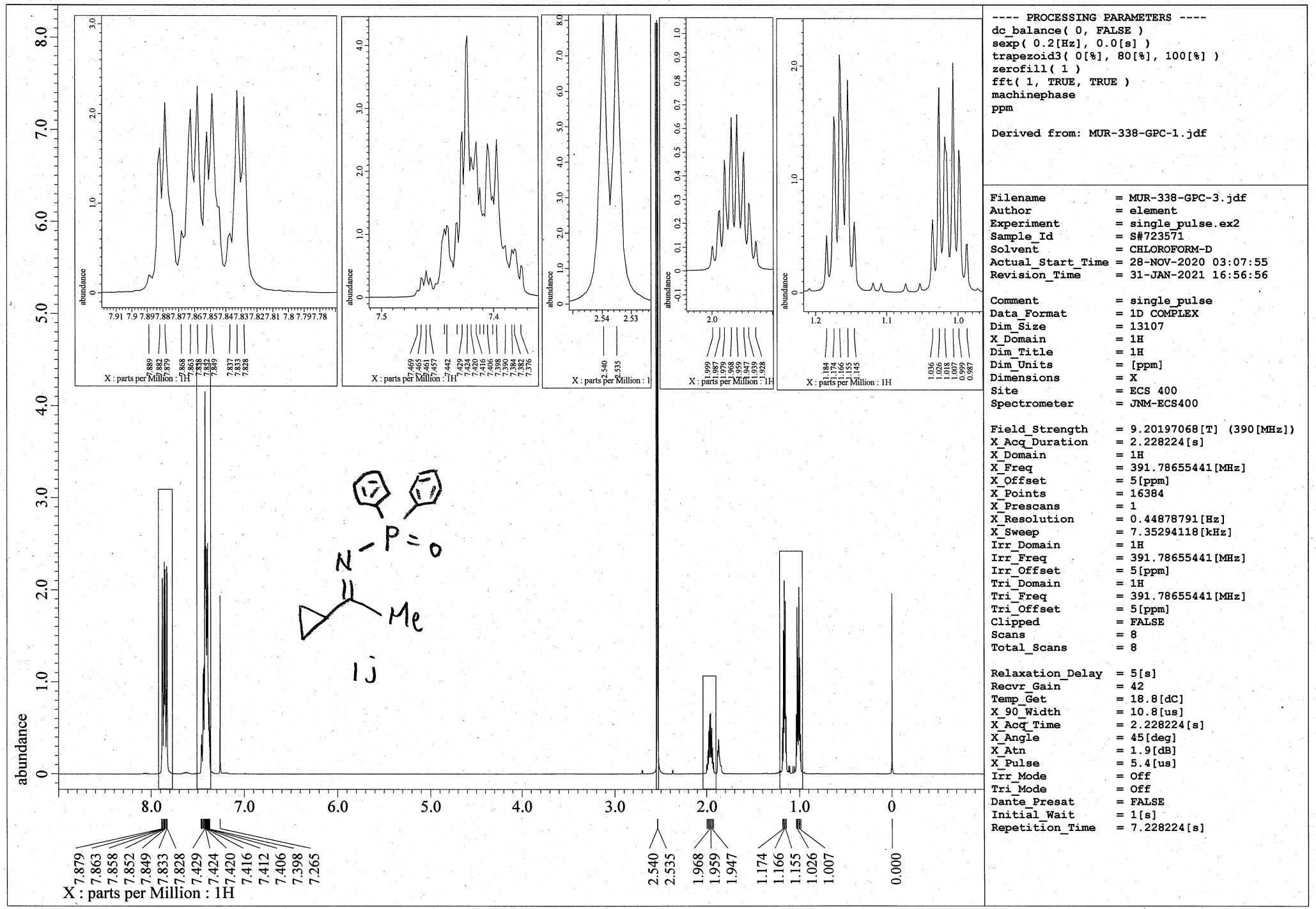

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-252-paper-13C-1.jdf
```

Filename	= MUR-252-paper-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-AUG-2020 01:35:15
Revision_Time	= 30-JAN-2021 20:02:44
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 300
Total_Scans	= 300
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 25.2[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]




```
---- 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: MUR-252-31P-1.jdf
```

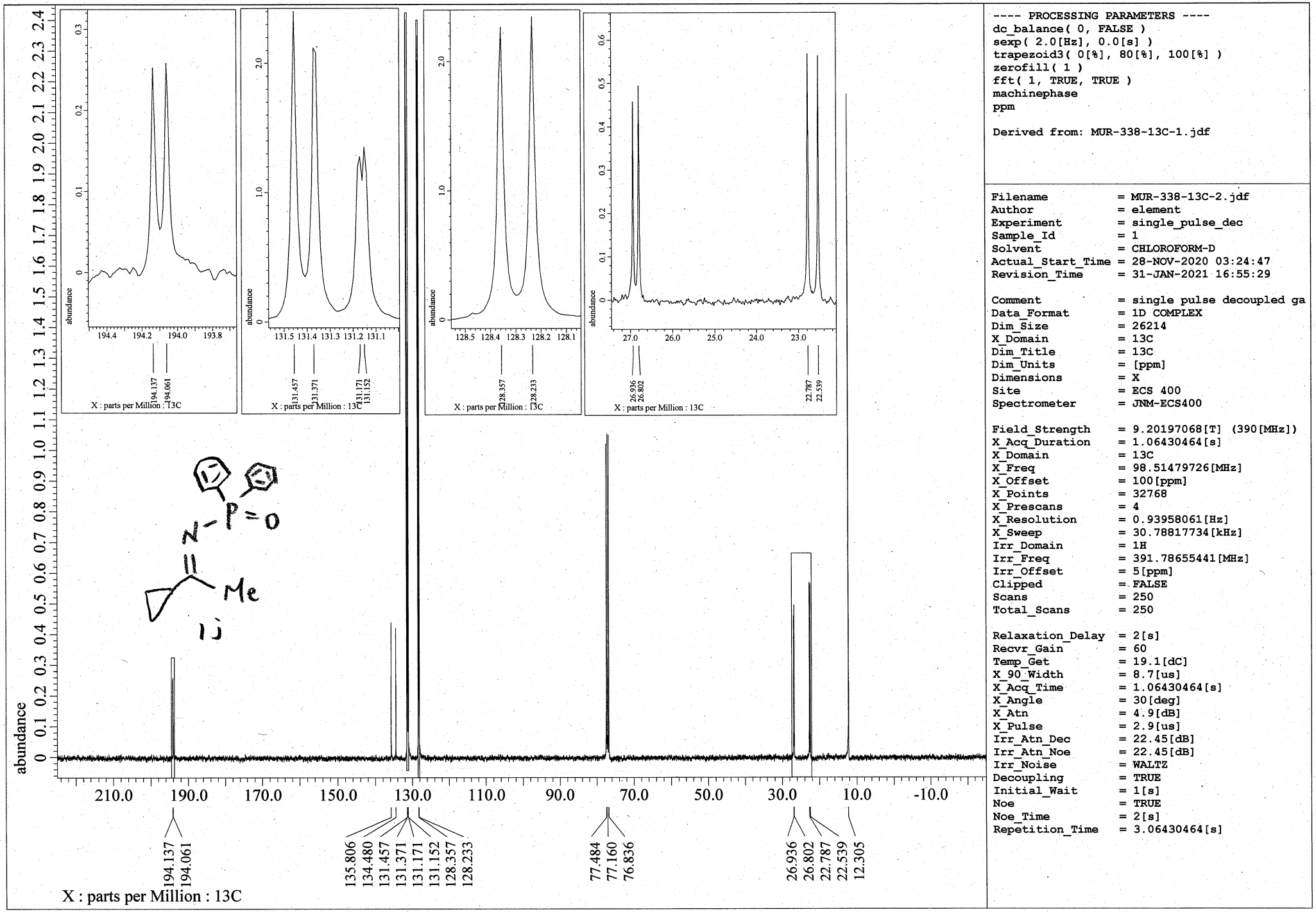
```
Filename            = MUR-252-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#443497
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-APR-2021 19:04:51
Revision_Time       =  6-MAY-2021 19:24:46

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[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

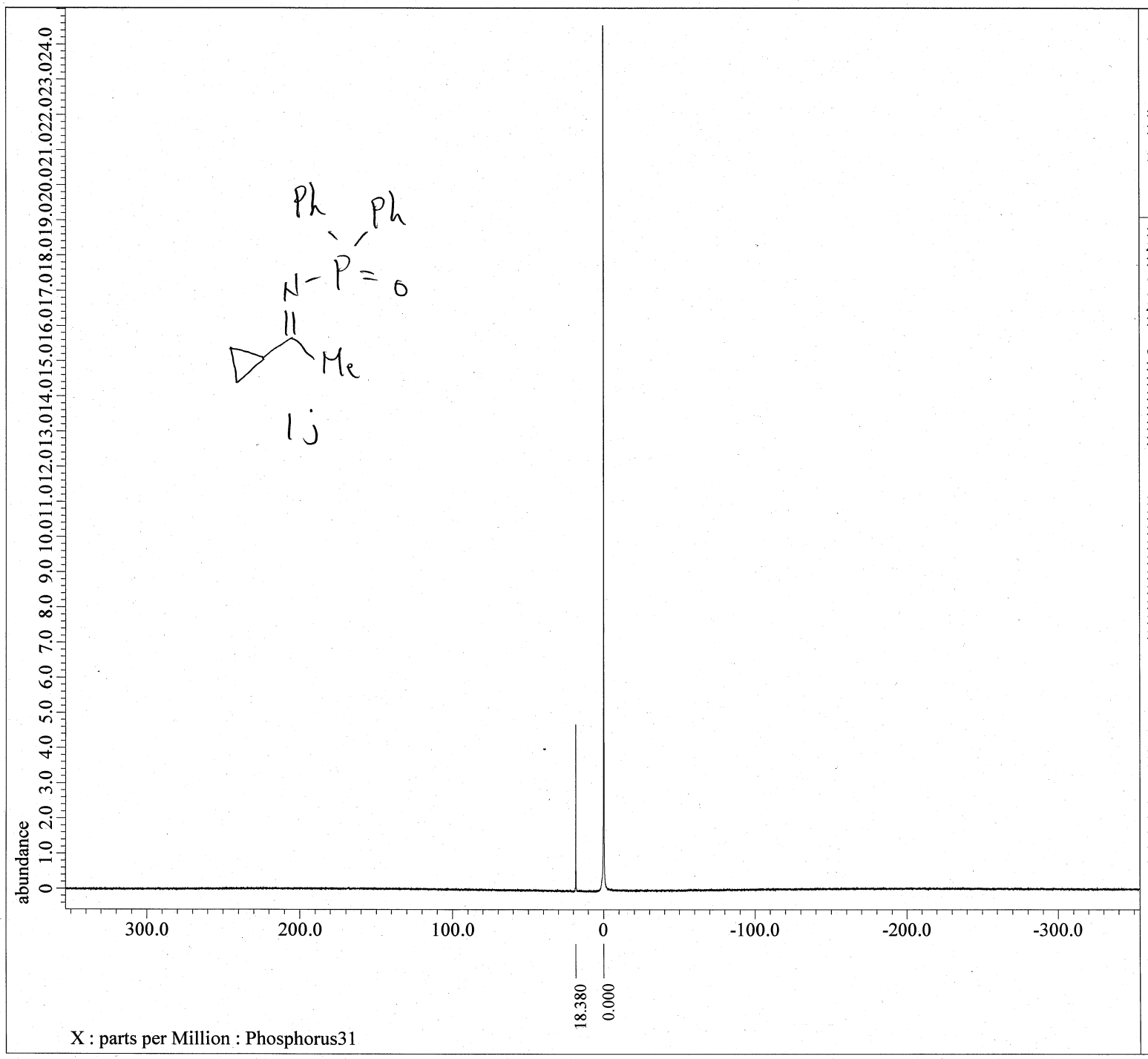
Derived from: MUR-338-GPC-1.jdf

Filename	= MUR-338-GPC-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#723571
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-NOV-2020 03:07:55
Revision_Time	= 31-JAN-2021 16:56:56
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	= 42
Temp_Get	= 18.8[dC]
X_90_Width	= 10.8[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]



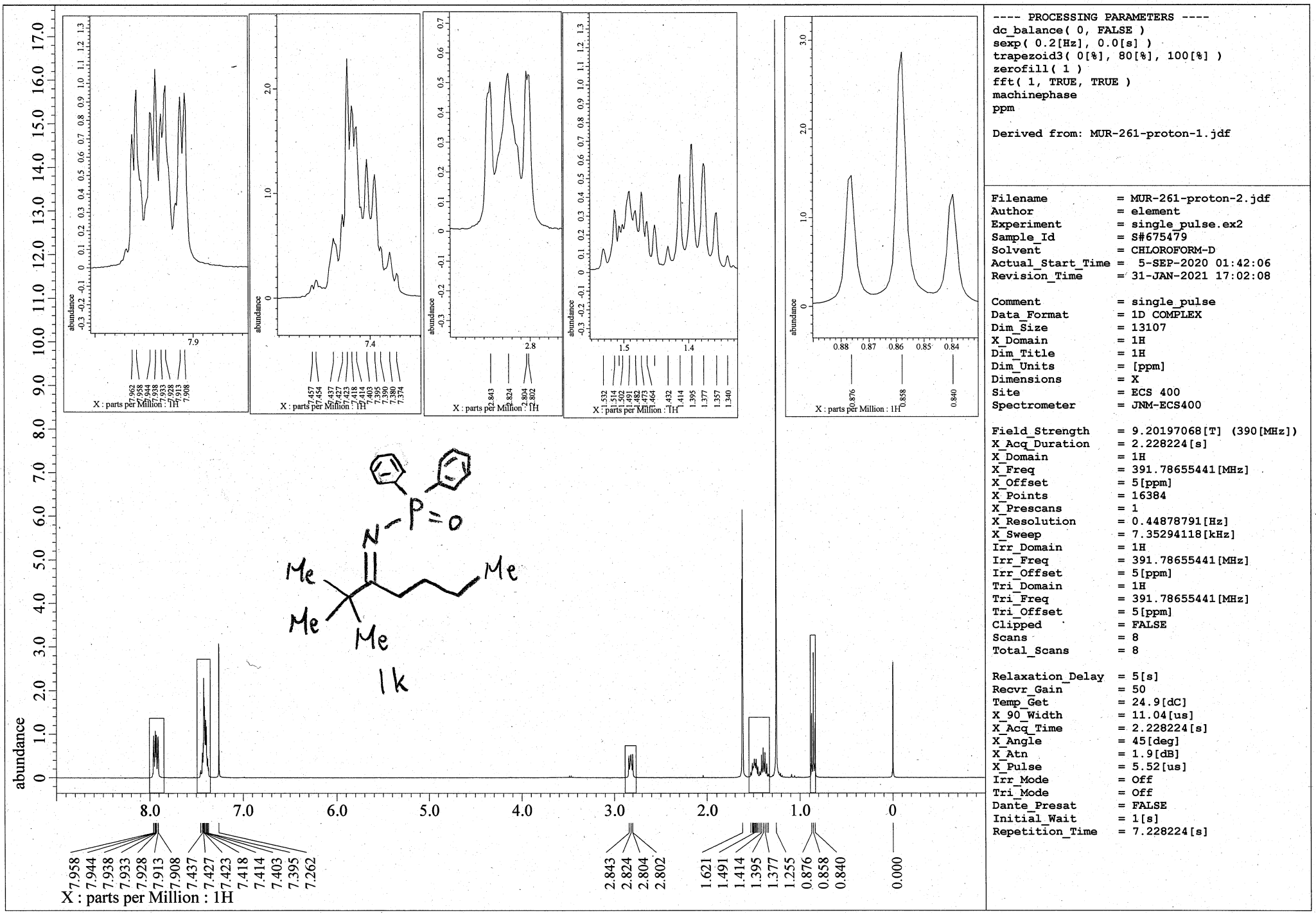

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-338-13C-1.jdf
```

Filename	= MUR-338-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-NOV-2020 03:24:47
Revision_Time	= 31-JAN-2021 16:55:29
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 250
Total_Scans	= 250
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.1[dC]
X_90_Width	= 8.7[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 2.9[us]
Irr_Atn_Dec	= 22.45[dB]
Irr_Atn_Noe	= 22.45[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



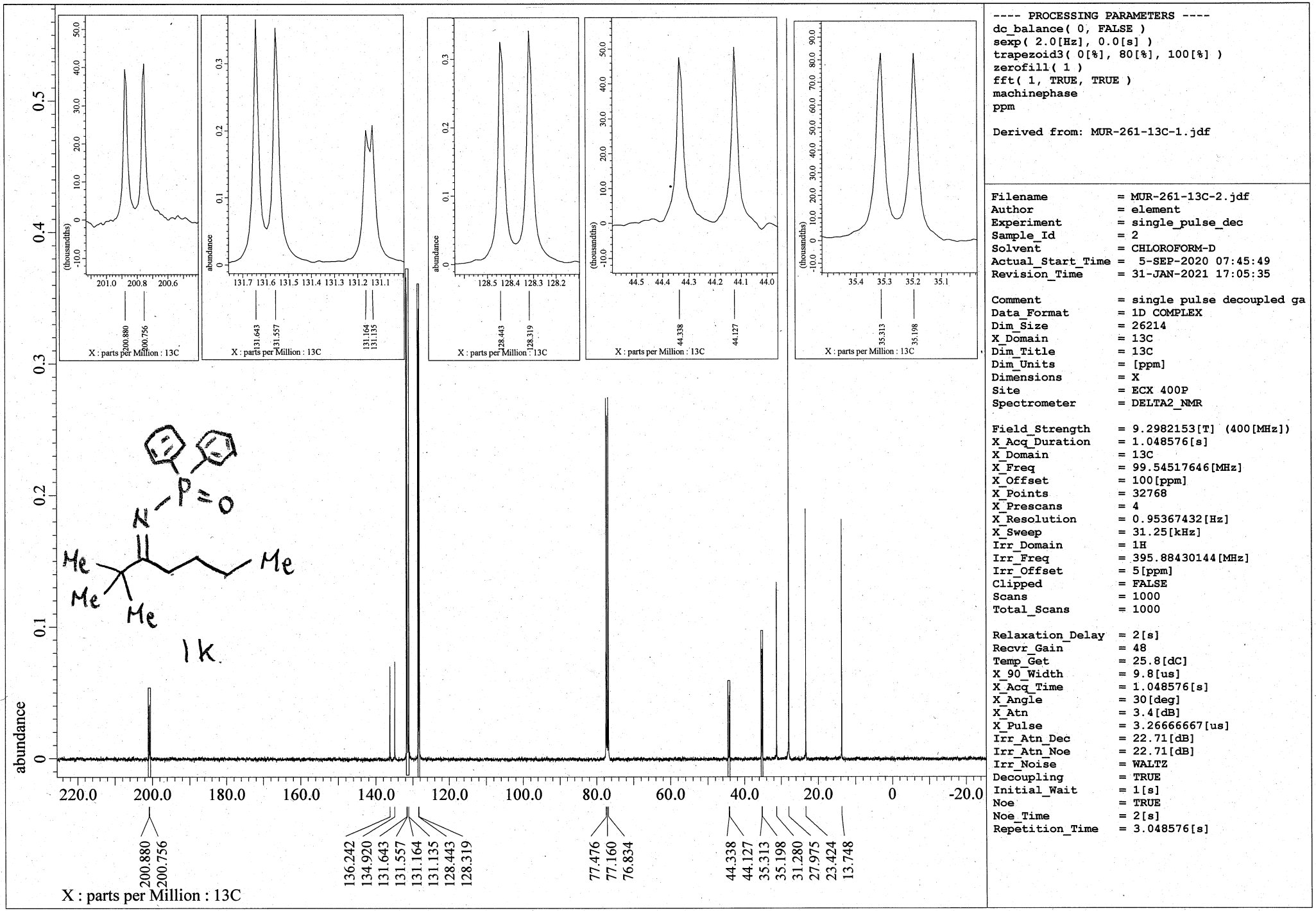

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-338-31P_Carbon-1-1.jdf
```

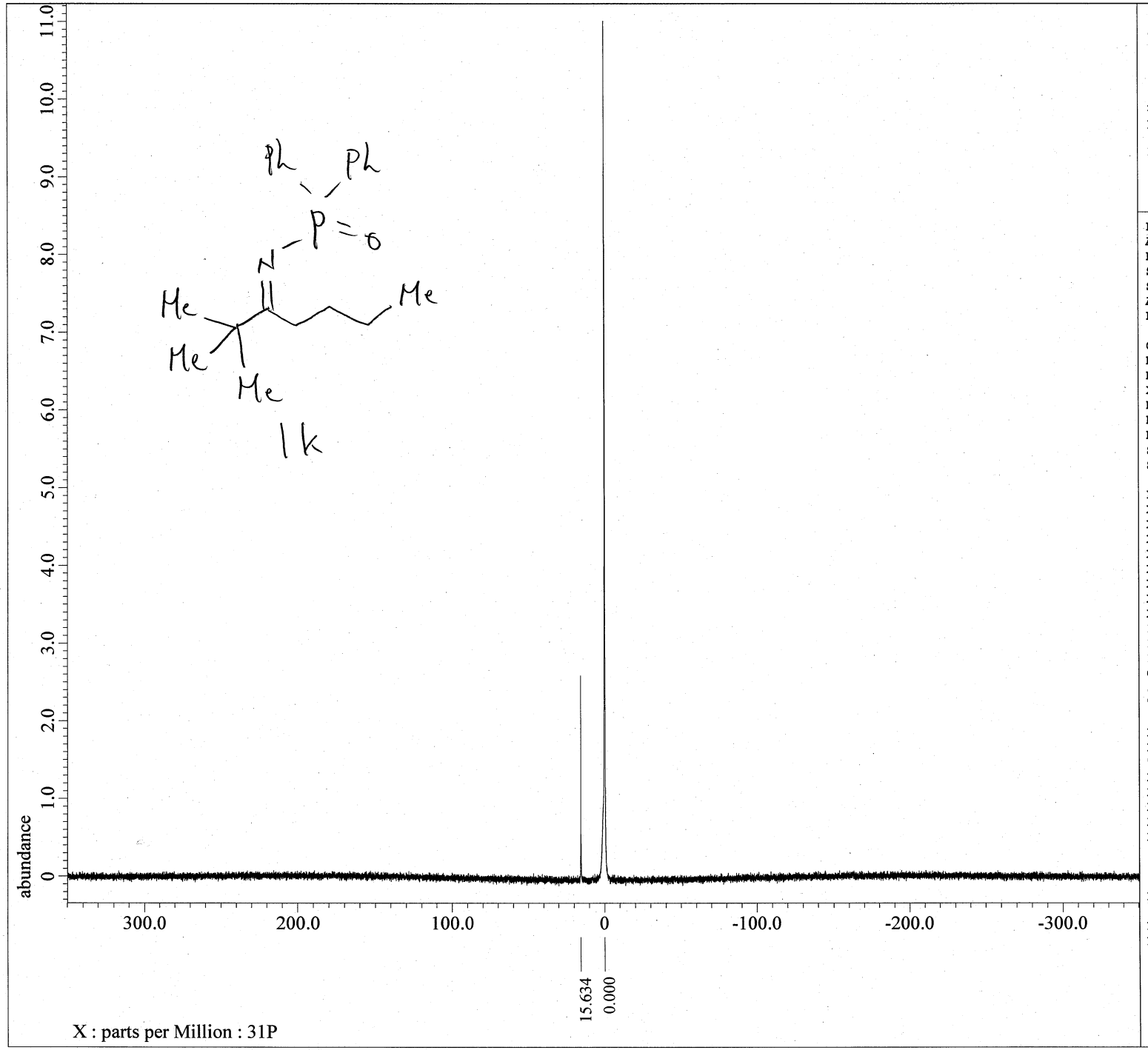
Filename	= MUR-338-31P_Carbon-1-2.jd
Author	= element
Experiment	= carbon.jxp
Sample_Id	= MUR-338-31P
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-APR-2021 14:44:36
Revision_Time	= 6-MAY-2021 19:30:35
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Phosph
Dim_Title	= Phosphorus31
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 0.229376[s]
X_Domain	= 31P
X_Freq	= 161.53211155[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 4.35965402[Hz]
X_Sweep	= 142.85714286[kHz]
X_Sweep_Clipped	= 114.28571429[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 20
Total_Scans	= 20
Relaxation_Delay	= 2[s]
Recvr_Gain	= 46
Temp_Get	= 18.5[dC]
X_90_Width	= 16.75[us]
X_Acq_Time	= 0.229376[s]
X_Angle	= 30[deg]
X_Atn	= 4.7[dB]
X_Pulse	= 5.58333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.229376[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

Derived from: MUR-261-proton-1.jdf
```

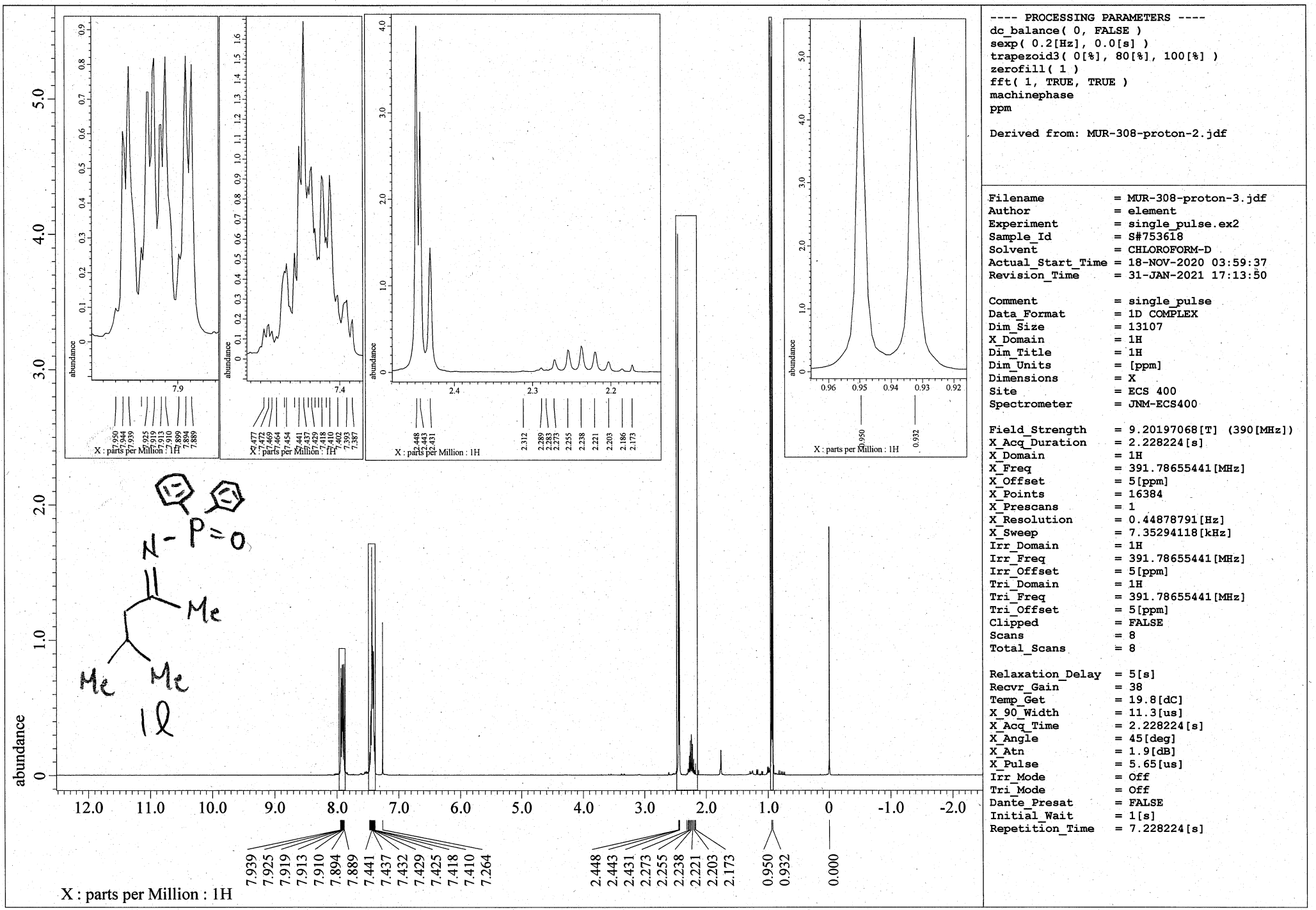
Filename	= MUR-261-proton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#675479
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-SEP-2020 01:42:06
Revision_Time	= 31-JAN-2021 17:02:08
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 24.9[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]


---- 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: MUR-261-13C-1.jdf
Filename = MUR-261-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 2
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2020 07:45:49
Revision_Time = 31-JAN-2021 17:05:35
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 25.8[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[s]
abundance
X : parts per Million : 13C
200.880
200.756
136.242
134.920
131.643
131.557
131.164
131.135
128.443
128.319
77.476
77.160
76.834
44.338
44.127
35.313
35.198
31.280
27.975
23.424
13.748
Me
Me
Me
Me
1k



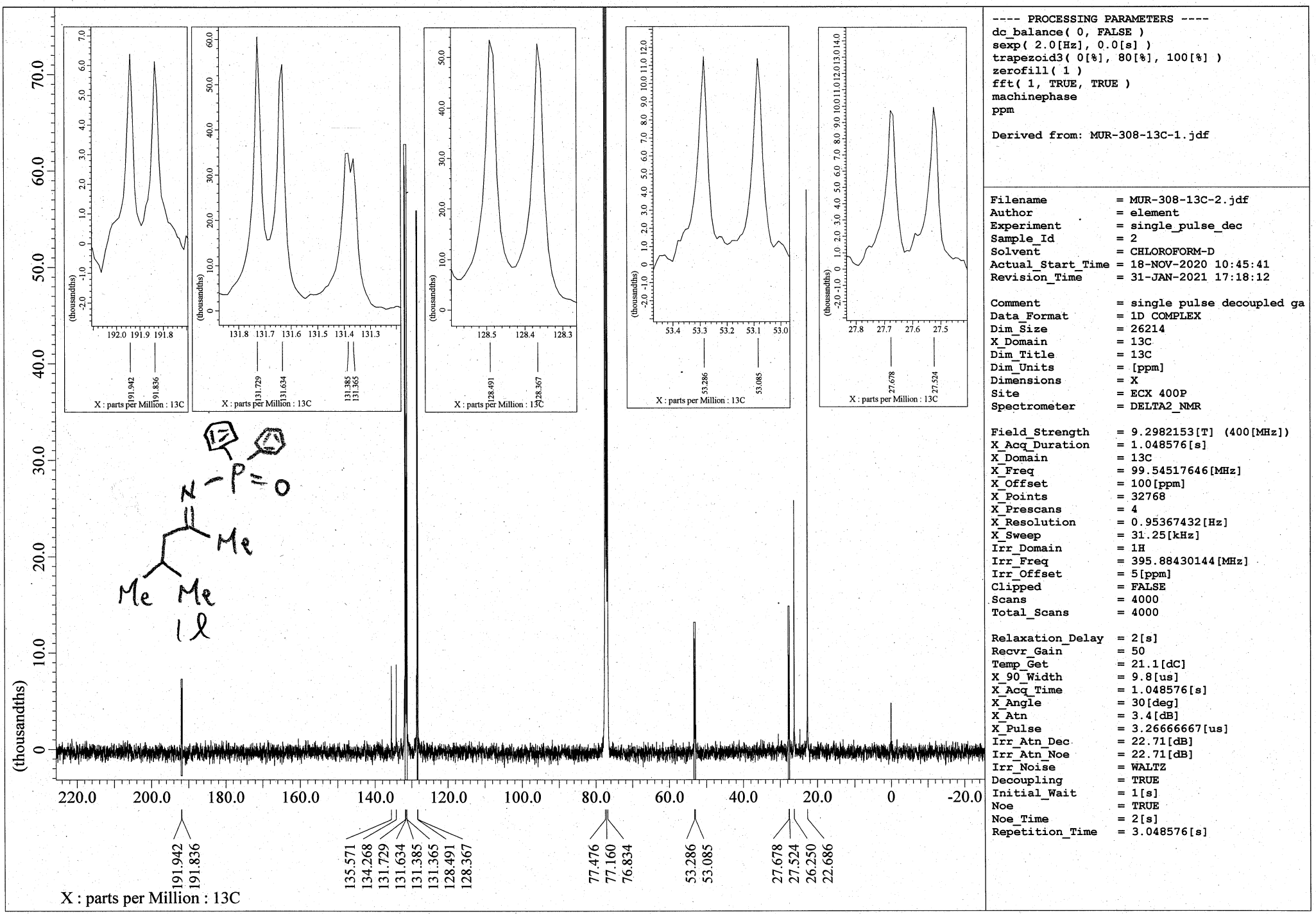

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-261-31P-1.jdf
```

```
Filename            = MUR-261-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#475611
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-APR-2021 19:58:25
Revision_Time       =  6-MAY-2021 19:27:03

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```



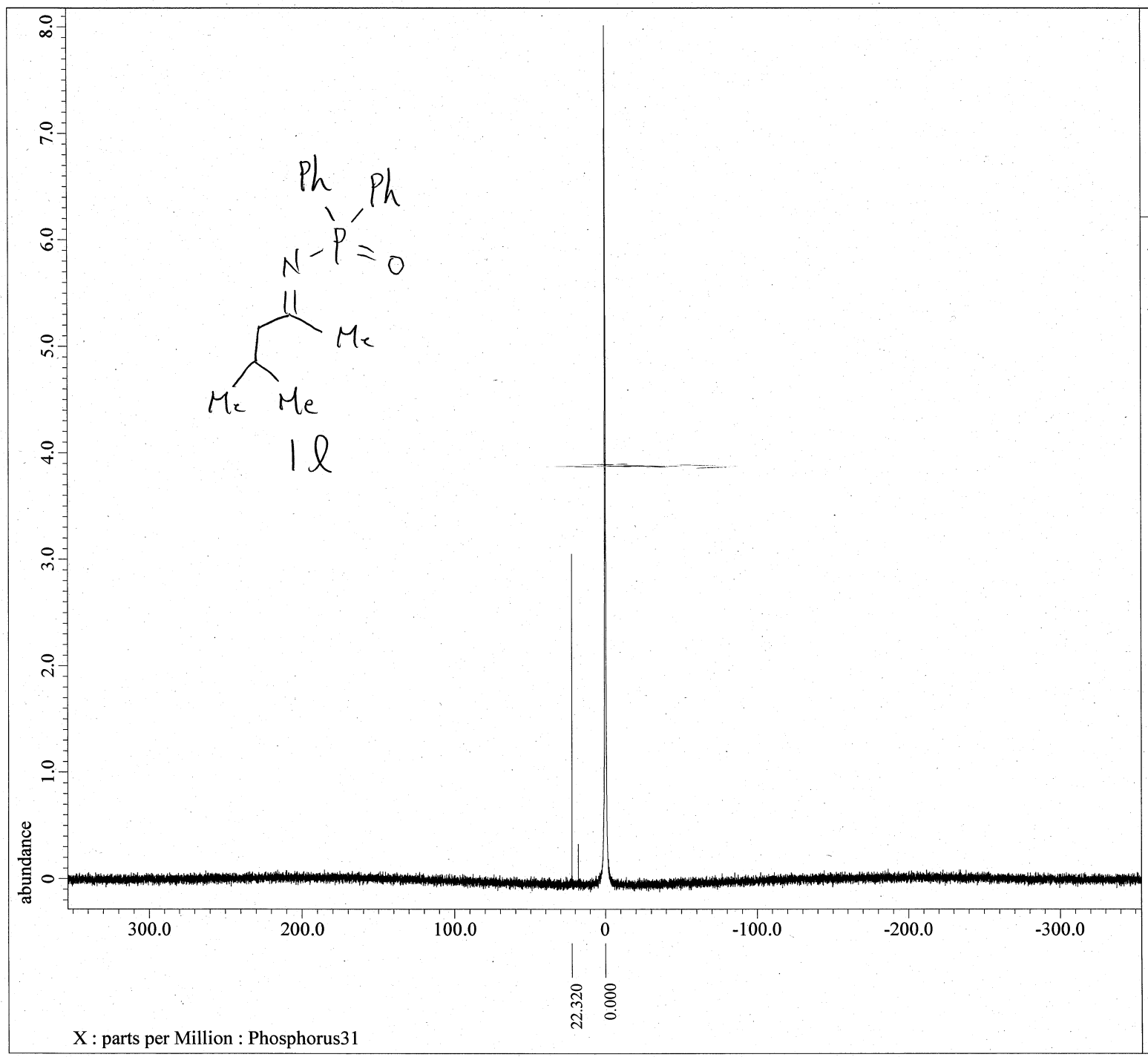

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-308-proton-2.jdf
```

Filename	= MUR-308-proton-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#753618
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-NOV-2020 03:59:37
Revision_Time	= 31-JAN-2021 17:13:50
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	= 38
Temp_Get	= 19.8[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]



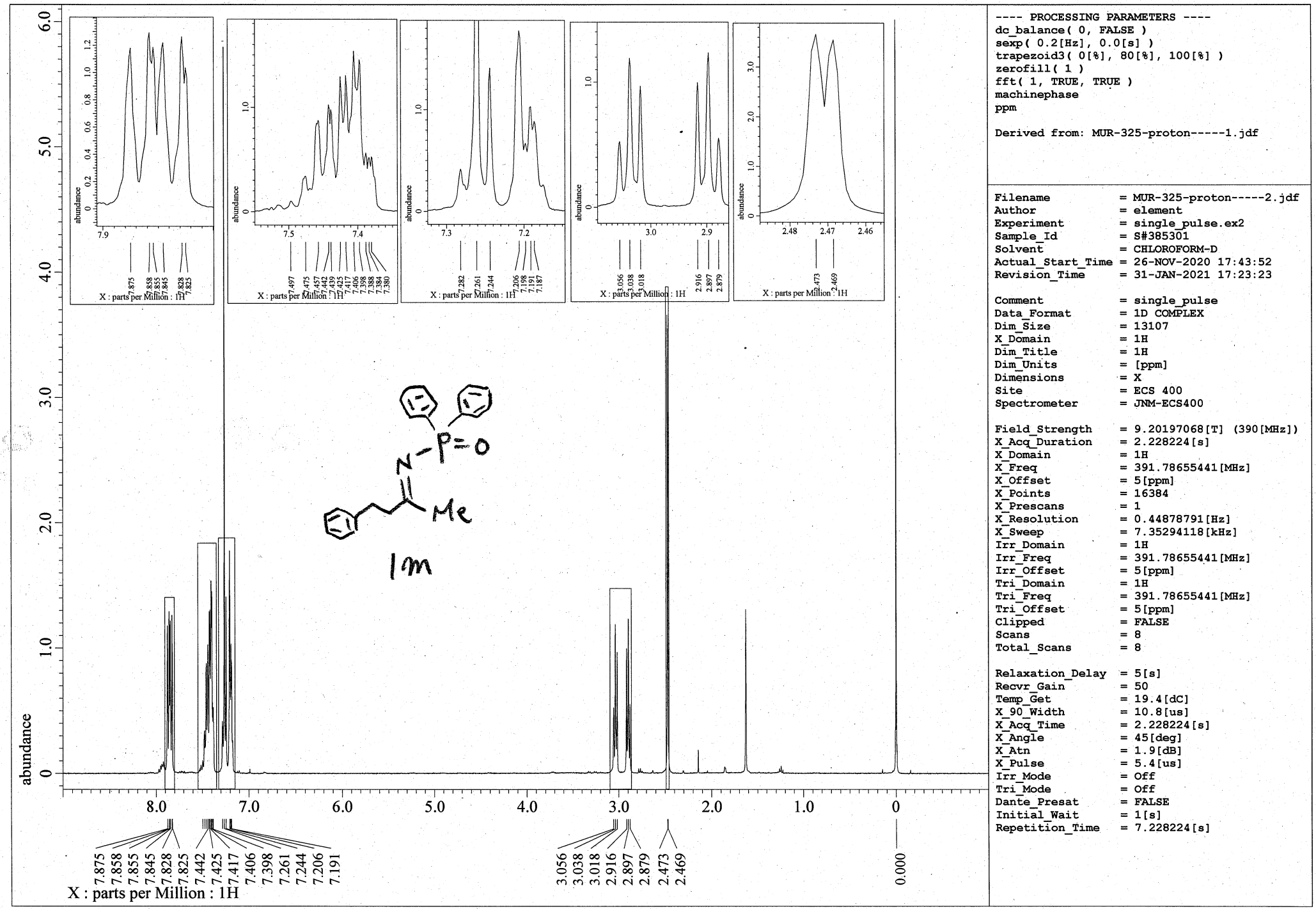

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-308-13C-1.jdf
```

Filename	= MUR-308-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-NOV-2020 10:45:41
Revision_Time	= 31-JAN-2021 17:18:12
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 1.048576[s]
X_Domain	= 13C
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 4000
Total_Scans	= 4000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.1[dC]
X_90_Width	= 9.8[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 3.26666667[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Atn_Noe	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.048576[s]



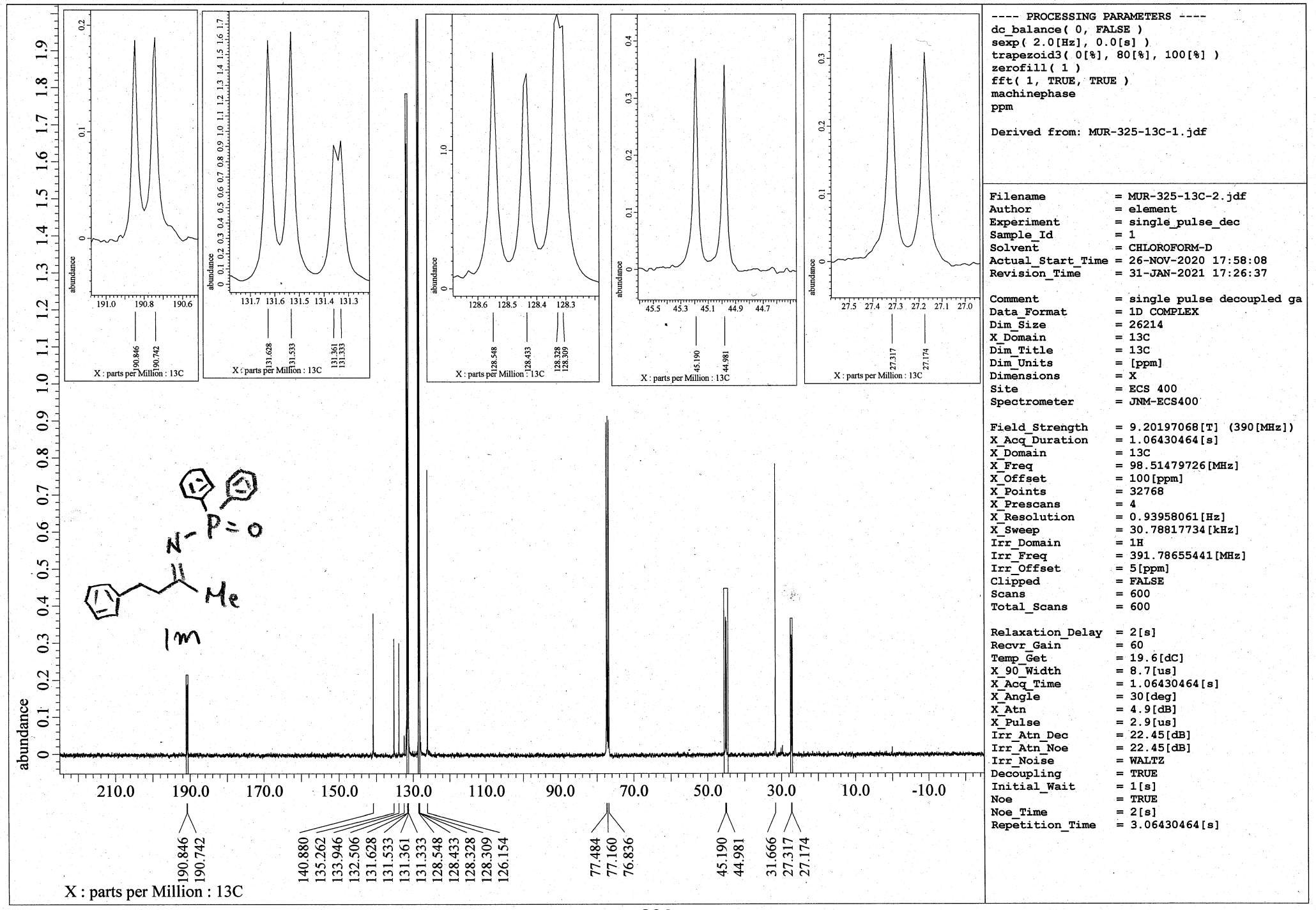

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-308-31P_Carbon-1-1.jdf
```

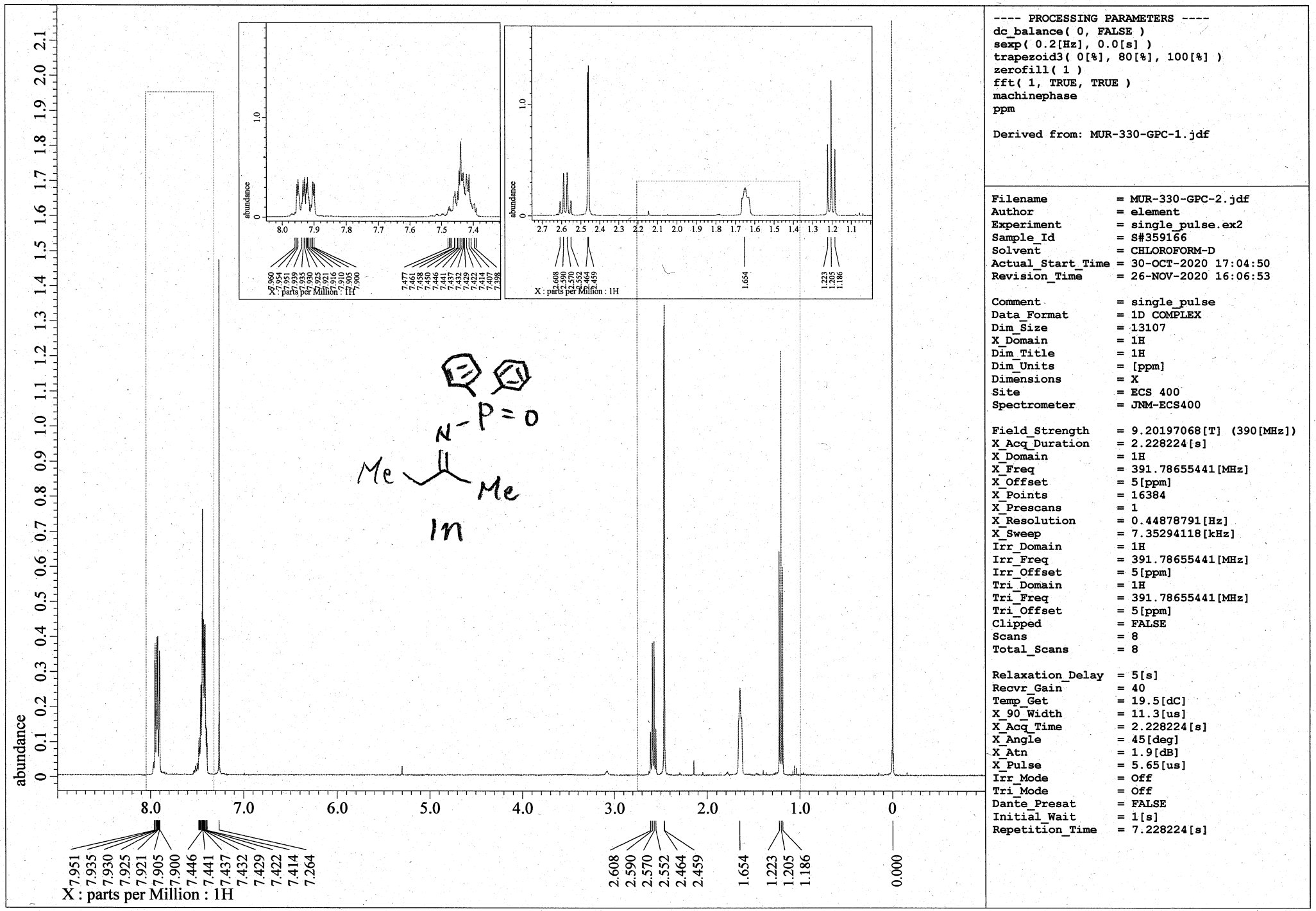
Filename	= MUR-308-31P_Carbon-1-2.jd
Author	= element
Experiment	= carbon.jxp
Sample_Id	= MUR-308-31P
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-APR-2021 14:51:22
Revision_Time	= 6-MAY-2021 19:28:21
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Phosph
Dim_Title	= Phosphorus31
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 0.229376[s]
X_Domain	= 31P
X_Freq	= 161.53211155[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 4.35965402[Hz]
X_Sweep	= 142.85714286[kHz]
X_Sweep_Clipped	= 114.28571429[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 20
Total_Scans	= 20
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.4[dC]
X_90_Width	= 16.75[us]
X_Acq_Time	= 0.229376[s]
X_Angle	= 30[deg]
X_Atn	= 4.7[dB]
X_Pulse	= 5.58333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.229376[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

Derived from: MUR-325-proton-----1.jdf
```

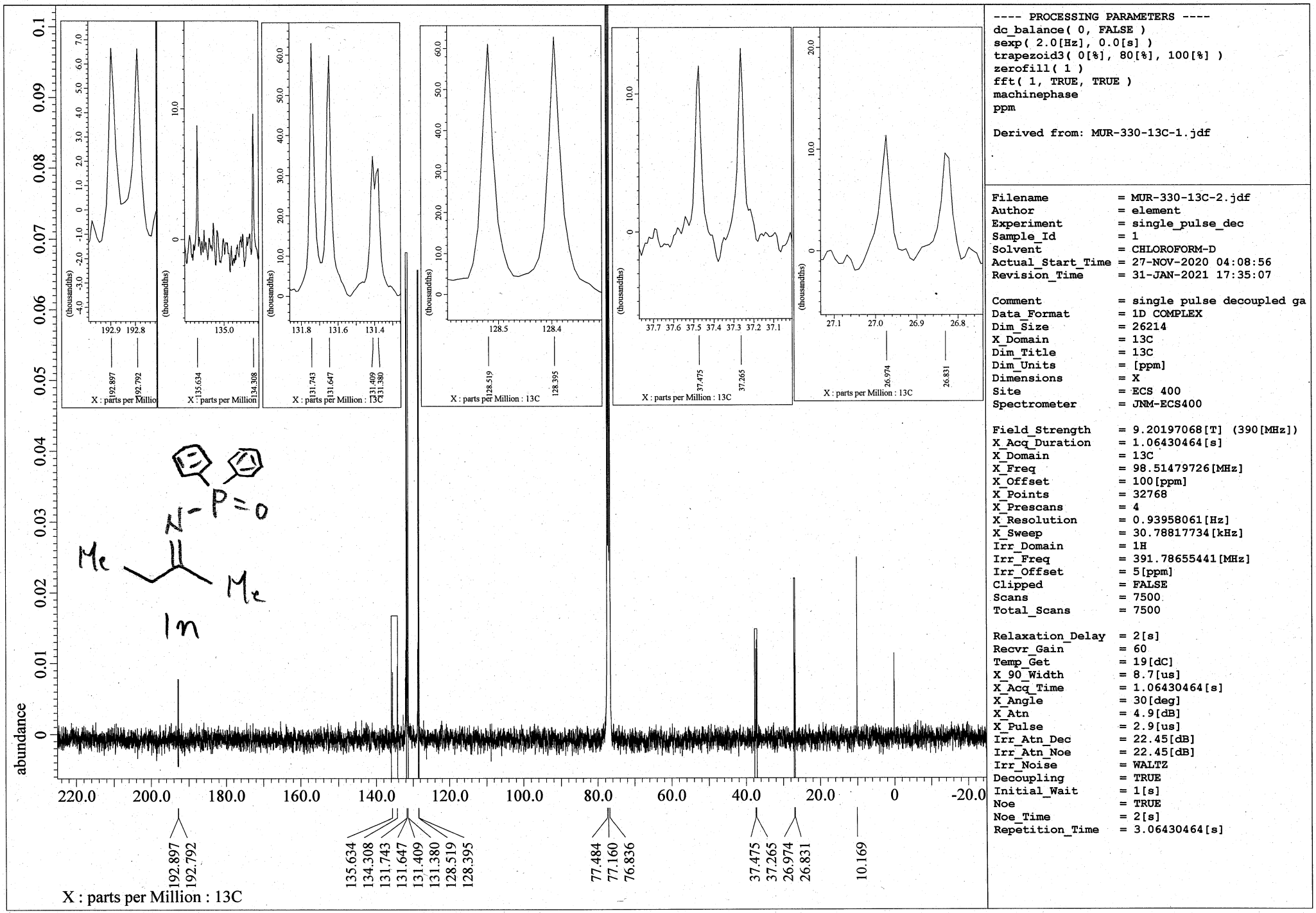
Filename	= MUR-325-proton-----2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#385301
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-NOV-2020 17:43:52
Revision_Time	= 31-JAN-2021 17:23:23
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 19.4[dC]
X_90_Width	= 10.8[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]

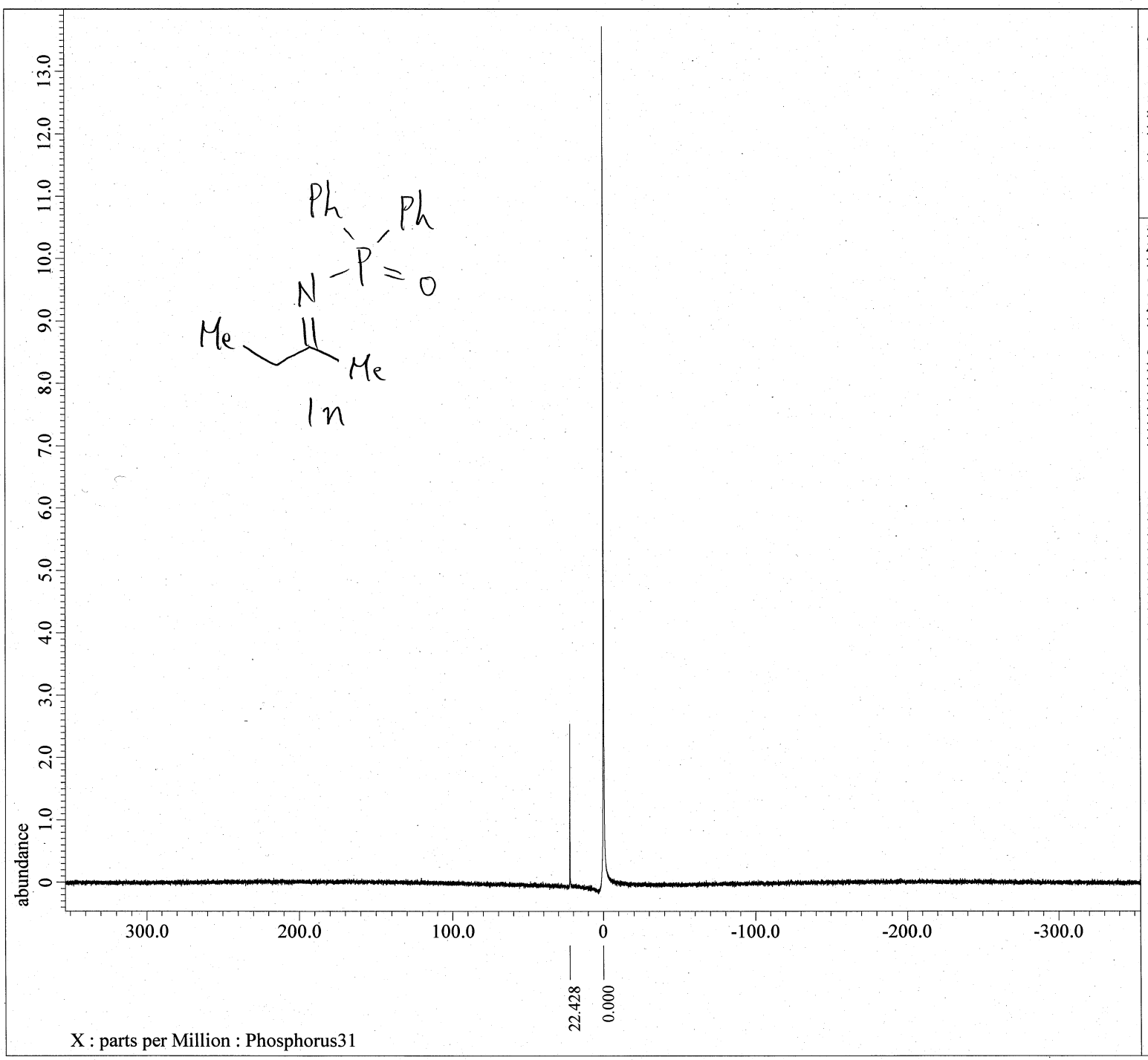

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-325-13C-1.jdf
Filename = MUR-325-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-NOV-2020 17:58:08
Revision_Time = 31-JAN-2021 17:26:37
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 600
Total_Scans = 600
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.6[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
N-P=O
Me
1m
abundance
X : parts per Million : 13C
190.846
190.742
140.880
135.262
133.946
132.506
131.628
131.533
131.361
131.333
128.548
128.433
128.328
128.309
126.154
77.484
77.160
76.836
45.190
44.981
31.666
27.317
27.174




```
---- 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: MUR-330-GPC-1.jdf
```

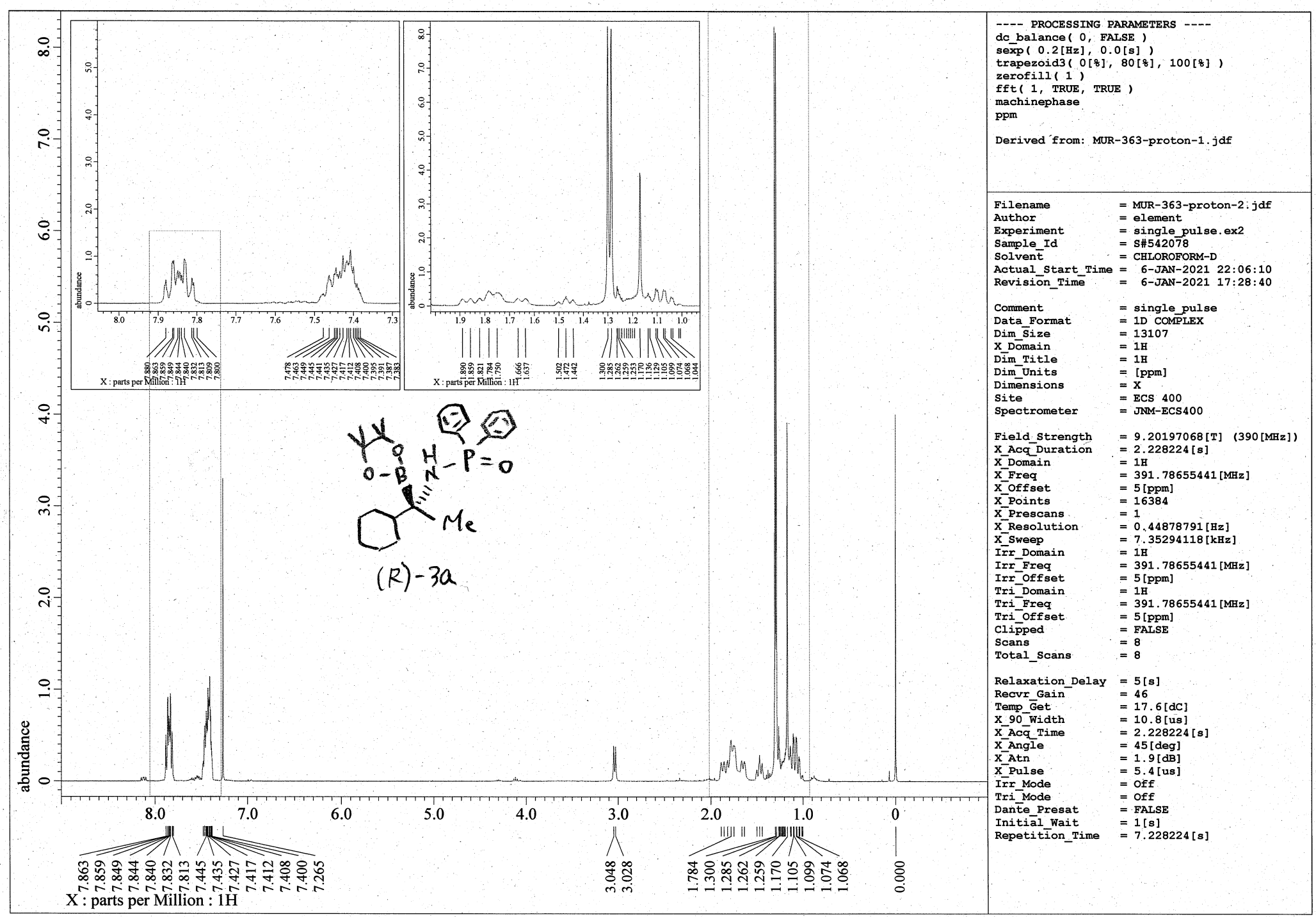
Filename	= MUR-330-GPC-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#359166
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-OCT-2020 17:04:50
Revision_Time	= 26-NOV-2020 16:06:53
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [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	= 40
Temp_Get	= 19.5[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]

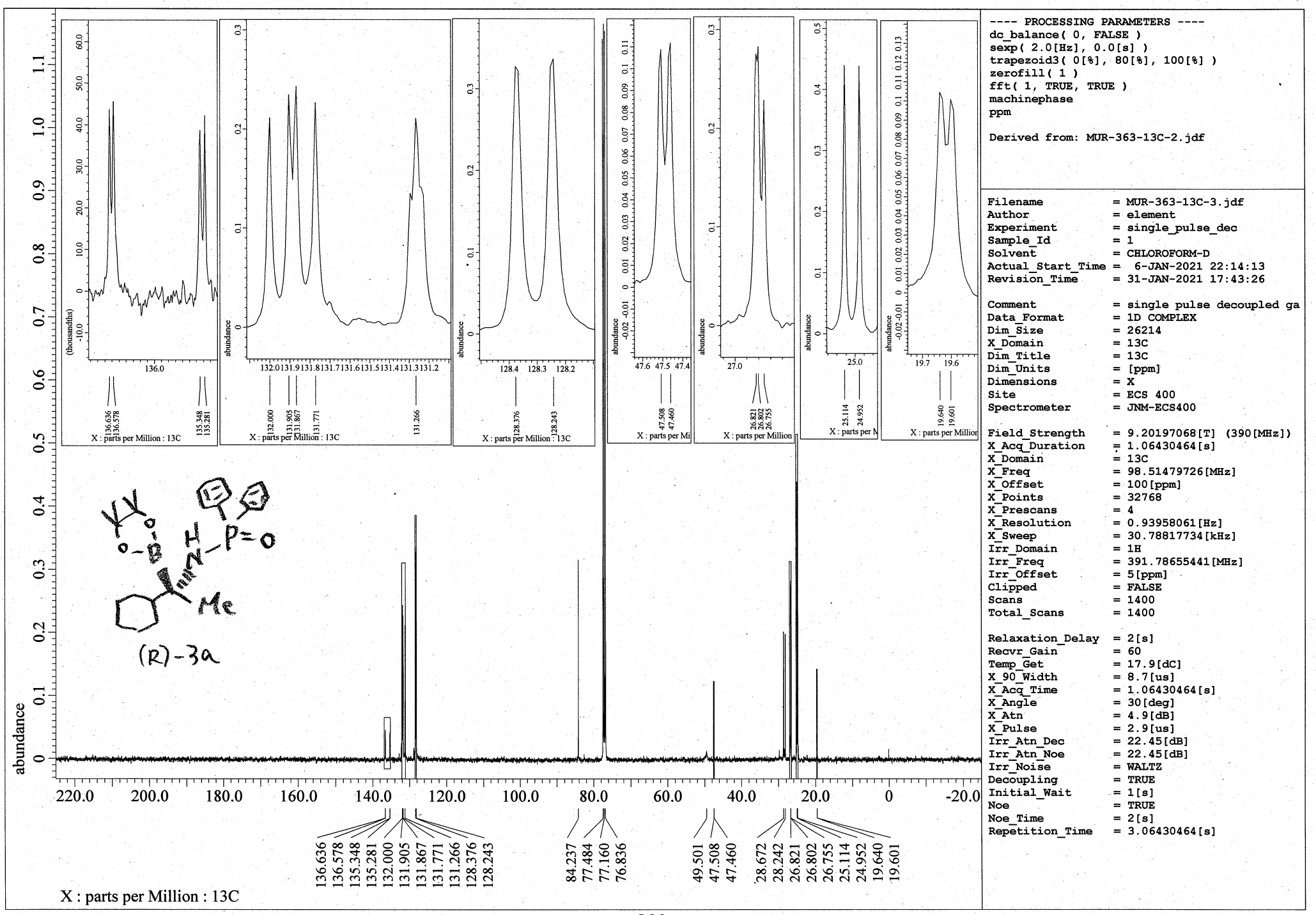

abundance
X : parts per Million : 13C
192.897
192.792
135.634
134.308
131.743
131.647
131.409
131.380
128.519
128.395
77.484
77.160
76.836
37.475
37.265
26.974
26.831
10.169
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-330-13C-1.jdf
Filename = MUR-330-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-NOV-2020 04:08:56
Revision_Time = 31-JAN-2021 17:35:07
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 7500
Total_Scans = 7500
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]




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

Derived from: MUR-330-31P_Carbon-1-1.jdf
```

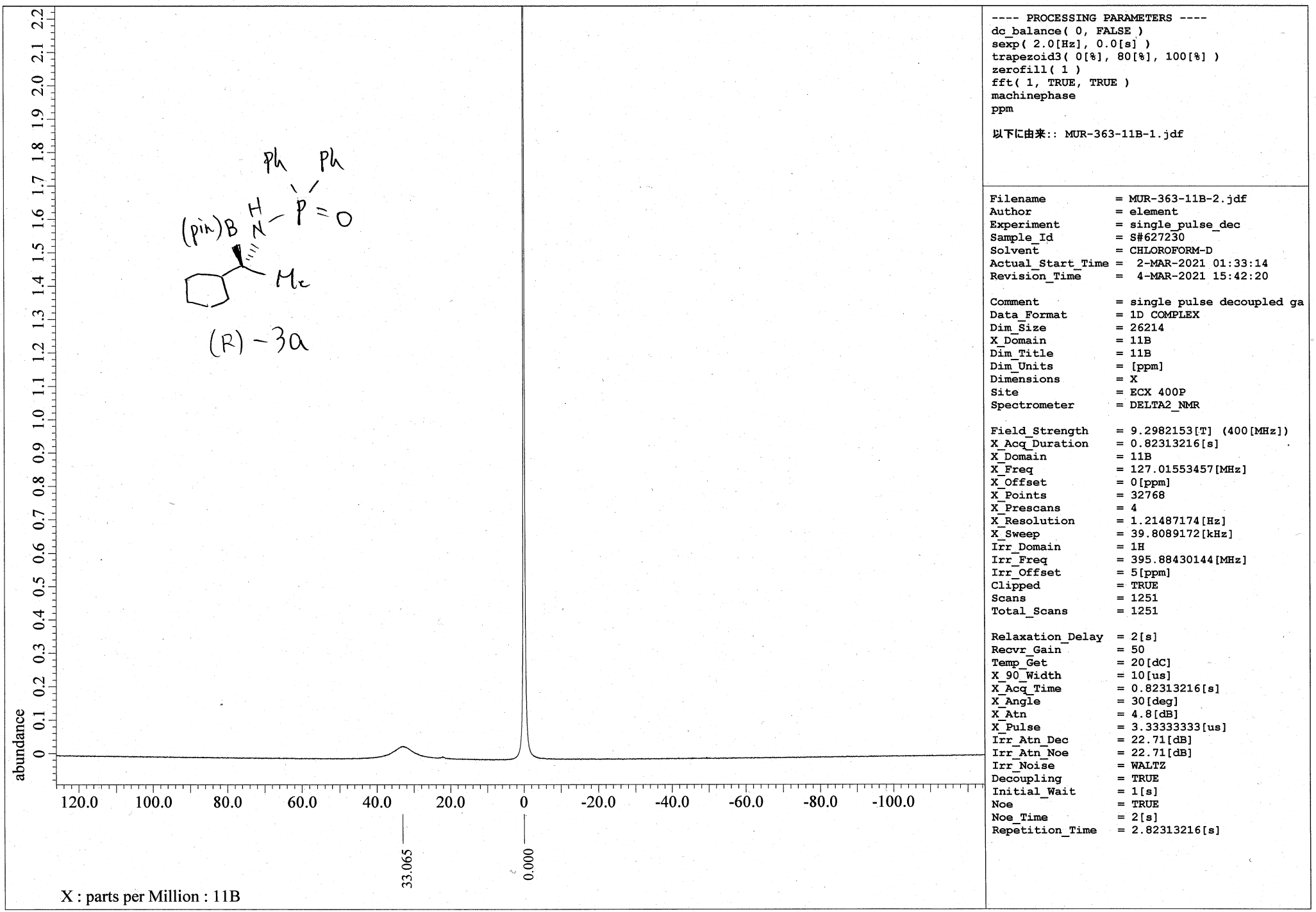
Filename	= MUR-330-31P_Carbon-1-2.jd
Author	= element
Experiment	= carbon.jxp
Sample_Id	= MUR-330-31P
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-APR-2021 14:58:47
Revision_Time	= 6-MAY-2021 19:30:10
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Phosph
Dim_Title	= Phosphorus31
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 0.229376[s]
X_Domain	= 31P
X_Freq	= 161.53211155[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 4.35965402[Hz]
X_Sweep	= 142.85714286[kHz]
X_Sweep_Clipped	= 114.28571429[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 20
Total_Scans	= 20
Relaxation_Delay	= 2[s]
Recvr_Gain	= 48
Temp_Get	= 18.3[dC]
X_90_Width	= 16.75[us]
X_Acq_Time	= 0.229376[s]
X_Angle	= 30[deg]
X_Atn	= 4.7[dB]
X_Pulse	= 5.58333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.229376[s]


abundance
X : parts per Million : 1H
7.863 7.859 7.849 7.844 7.840 7.832 7.813 7.445 7.435 7.427 7.417 7.412 7.408 7.400 7.265
3.048 3.028
1.784 1.300 1.285 1.262 1.259 1.170 1.105 1.099 1.074 1.068
0.000
(R)-3a
---- 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: MUR-363-proton-1.jdf
Filename = MUR-363-proton-2.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#542078
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-JAN-2021 22:06:10
Revision_Time = 6-JAN-2021 17:28:40
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 2.228224[s]
X_Domain = 1H
X_Freq = 391.78655441[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.44878791[Hz]
X_Sweep = 7.35294118[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 391.78655441[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 17.6[dC]
X_90_Width = 10.8[us]
X_Acq_Time = 2.228224[s]
X_Angle = 45[deg]
X_Atn = 1.9[dB]
X_Pulse = 5.4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.228224[s]



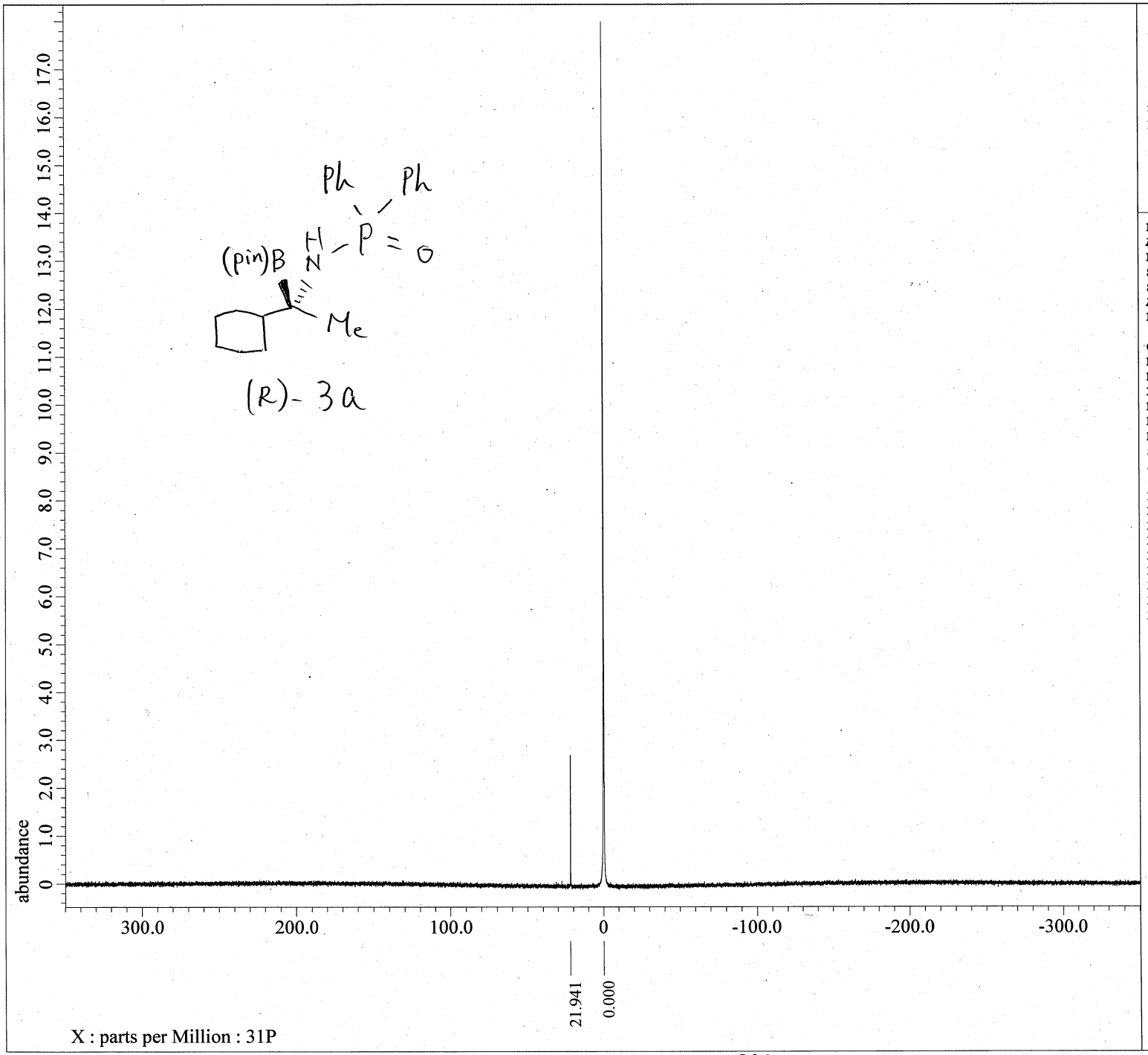

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-363-13C-2.jdf
```

Filename	= MUR-363-13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-JAN-2021 22:14:13
Revision_Time	= 31-JAN-2021 17:43:26
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1400
Total_Scans	= 1400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 17.9[dC]
X_90_Width	= 8.7[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 2.9[us]
Irr_Atn_Dec	= 22.45[dB]
Irr_Atn_Noe	= 22.45[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



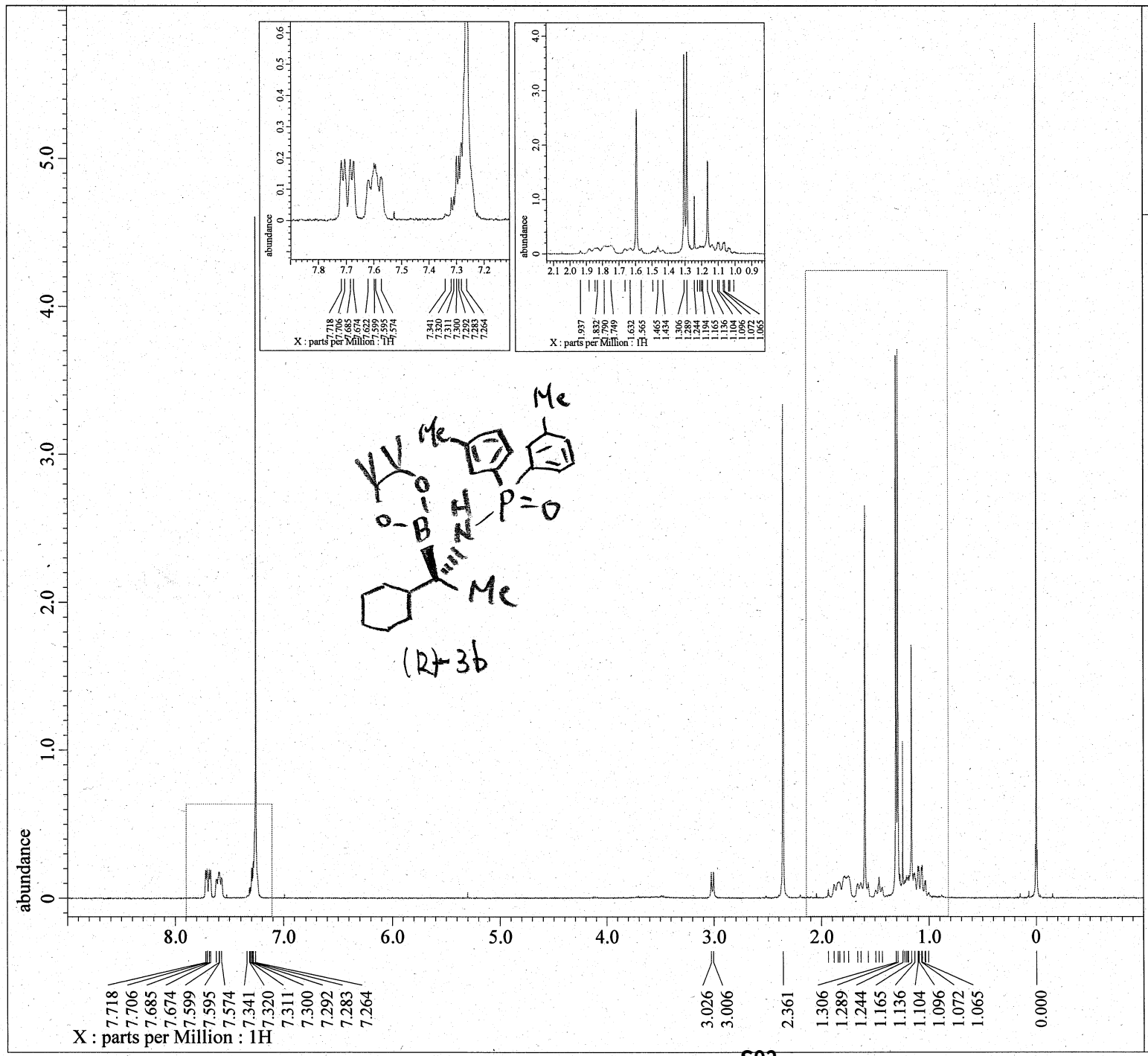

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-363-11B-1.jdf
```

```
Filename            = MUR-363-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#627230
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  2-MAR-2021 01:33:14
Revision_Time       =  4-MAR-2021 15:42:20

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = TRUE
Scans               = 1251
Total_Scans         = 1251

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```



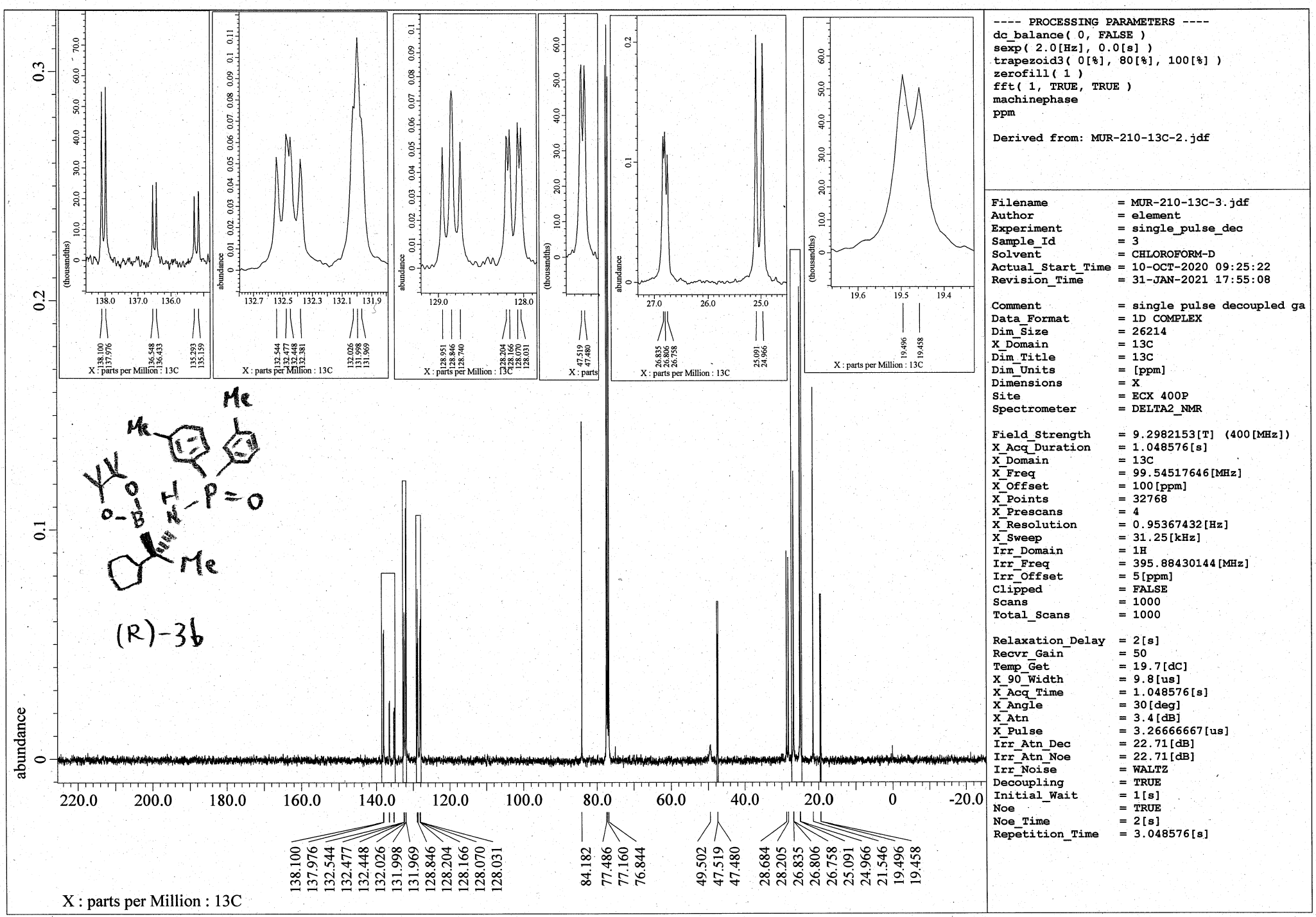

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-363-31P-1.jdf
```

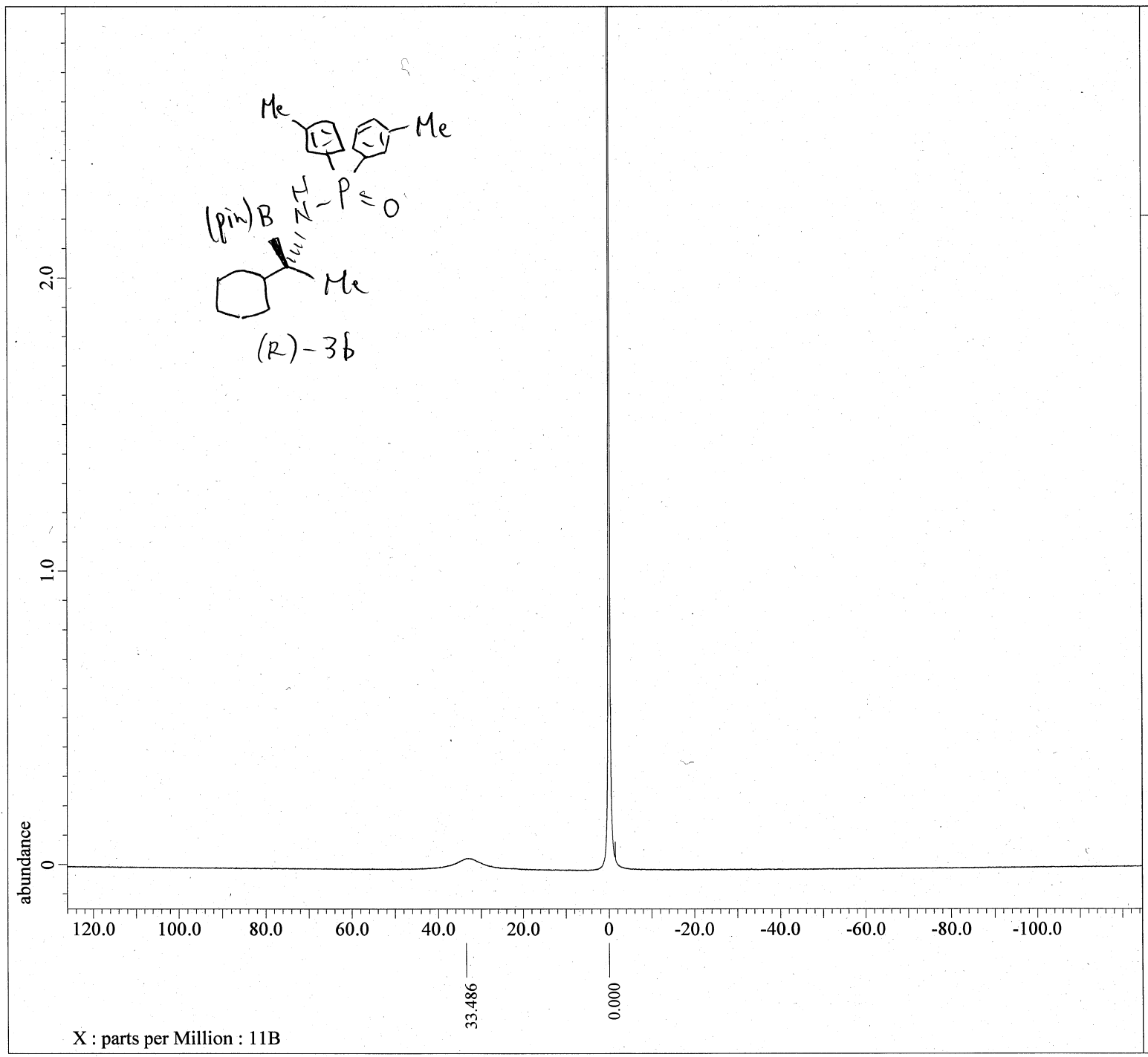
```
Filename            = MUR-363-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#447973
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 19:12:26
Revision_Time       =  6-MAY-2021 21:31:32

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.2[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[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

Derived from: MUR-210-proton-1.jdf
```

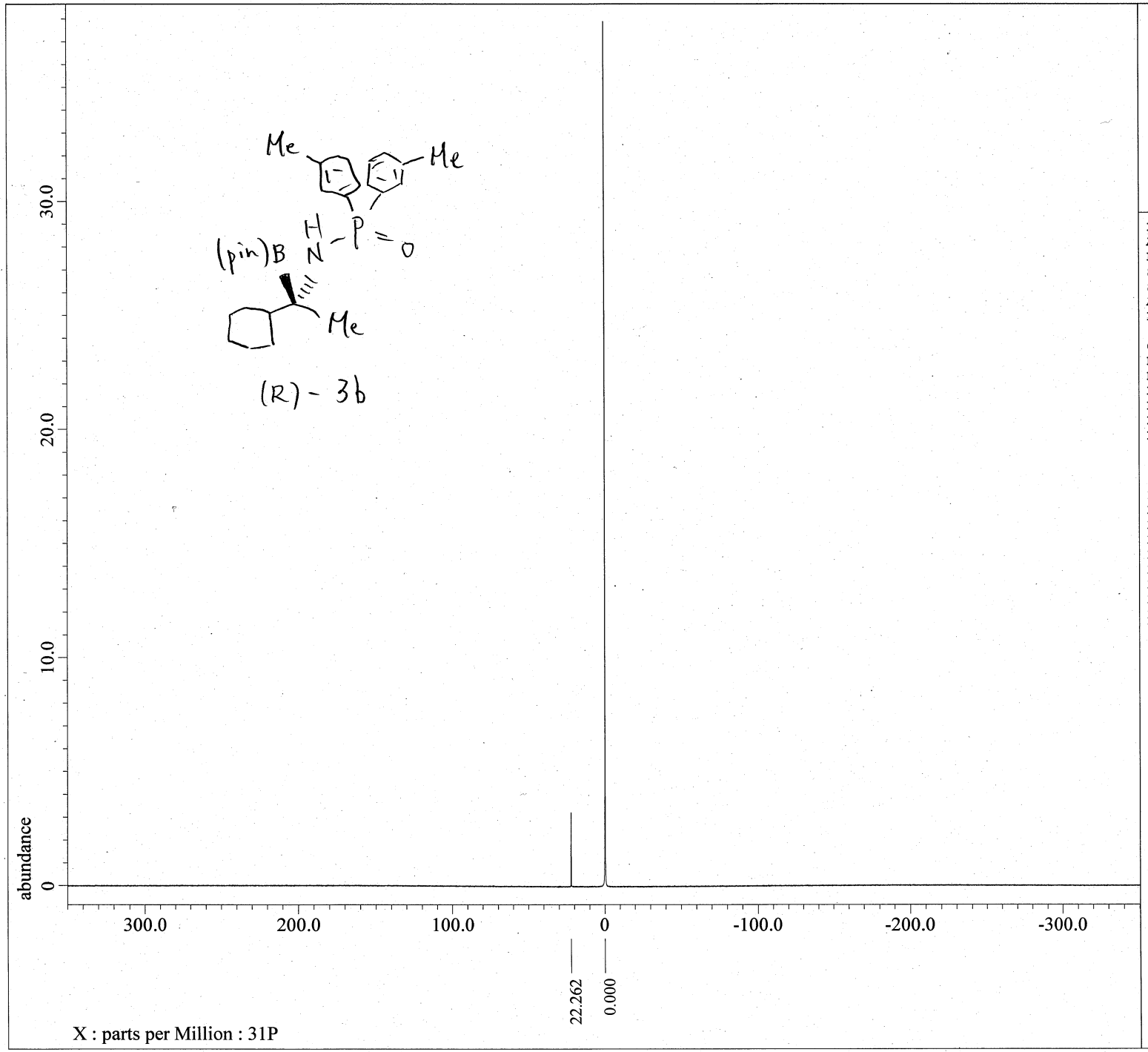
Filename	= MUR-210-proton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#566172
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-OCT-2020 22:50:53
Revision_Time	= 21-OCT-2020 10:19:12
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 20.5[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]


---- 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: MUR-210-13C-2.jdf
Filename = MUR-210-13C-3.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 3
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-OCT-2020 09:25:22
Revision_Time = 31-JAN-2021 17:55:08
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.7[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[s]
Me
Me
Me
(R)-3b
abundance
X : parts per Million : 13C
138.100
137.976
132.544
132.477
132.448
132.026
131.998
131.969
128.846
128.204
128.166
128.070
128.031
84.182
77.486
77.160
76.844
49.502
47.519
47.480
28.684
28.205
26.835
26.806
26.758
25.091
24.966
21.546
19.496
19.458



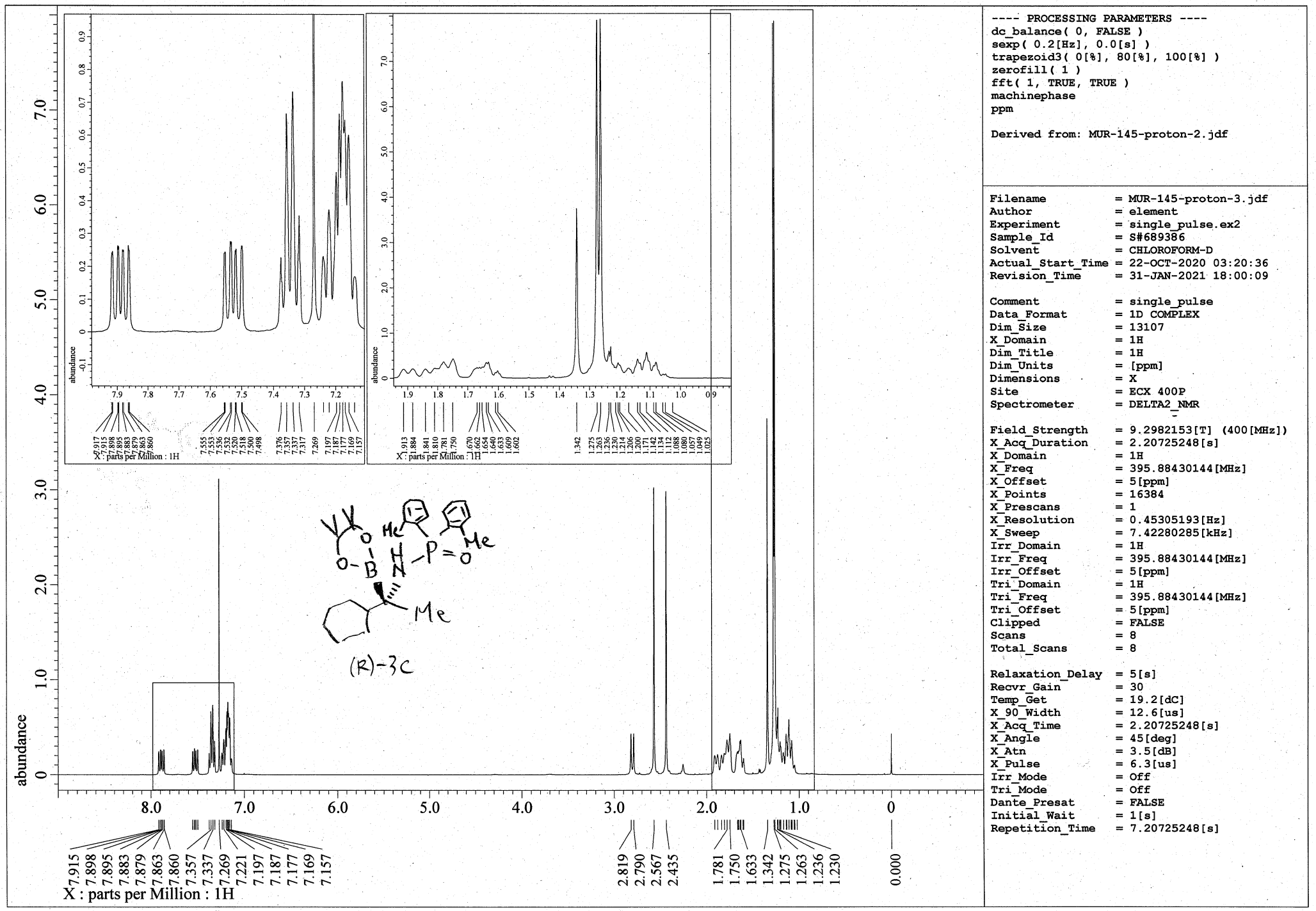

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-210-11B-1.jdf
```

```
Filename            = MUR-210-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#707931
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  2-MAR-2021 03:47:23
Revision_Time       =  4-MAR-2021 15:33:27

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 1000
Total_Scans         = 1000

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.6[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```



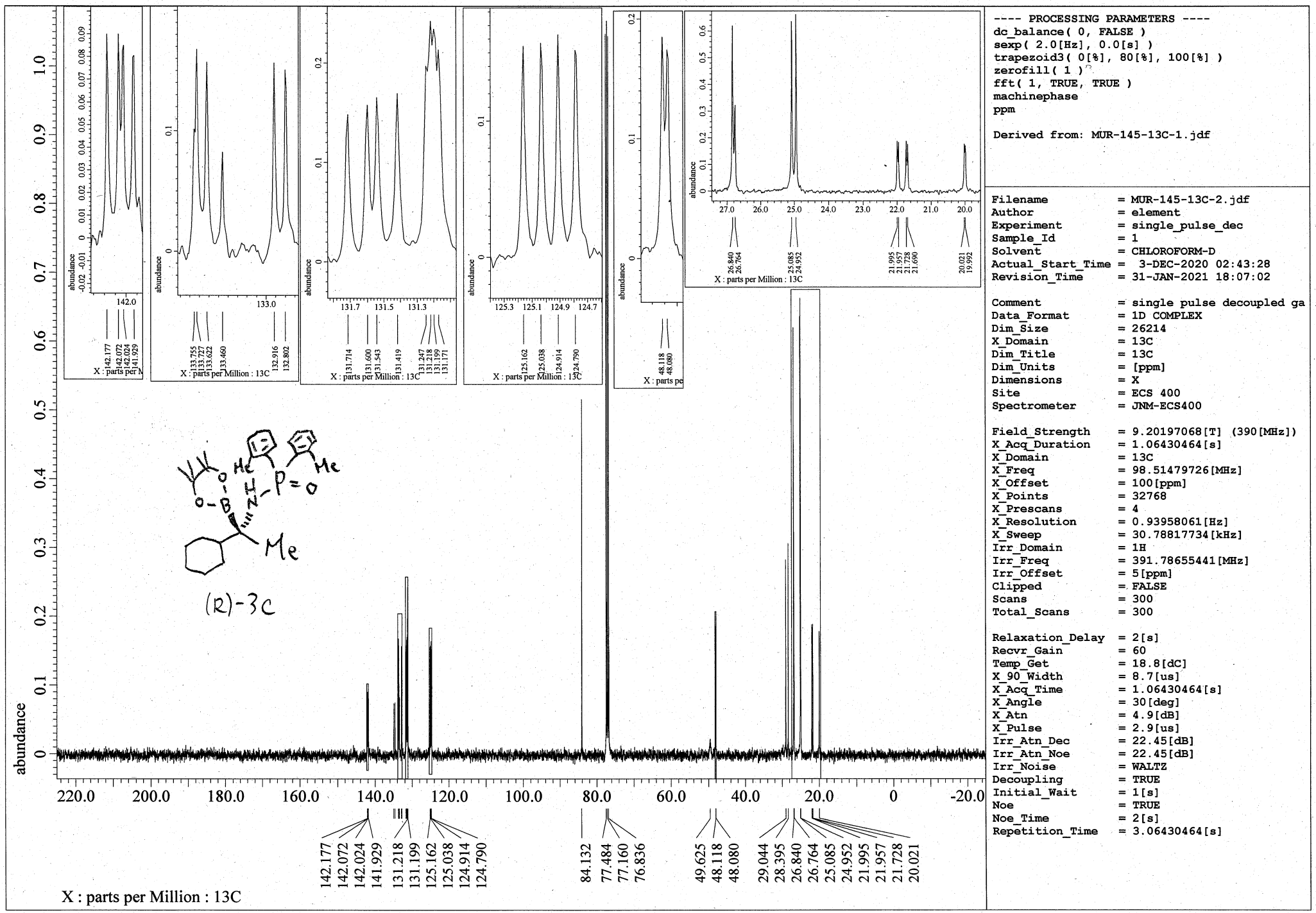

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-210-31P-1.jdf
```

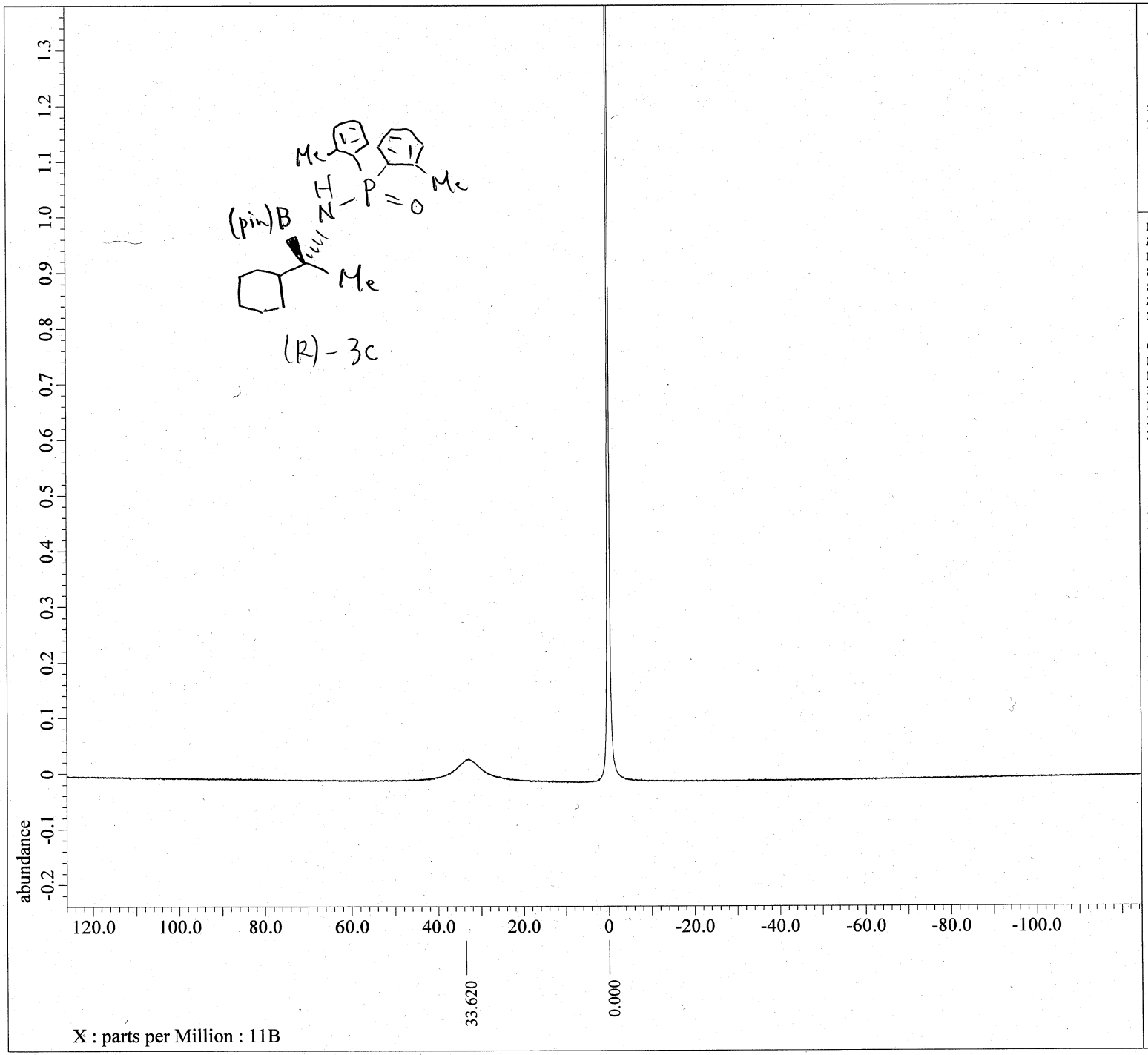
```
Filename            = MUR-210-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#426339
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 18:36:29
Revision_Time       =  6-MAY-2021 21:28:03

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 50
Total_Scans         = 50

Relaxation_Delay    = 2[s]
Recvr_Gain          = 48
Temp_Get            = 19[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[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

Derived from: MUR-145-proton-2.jdf
```

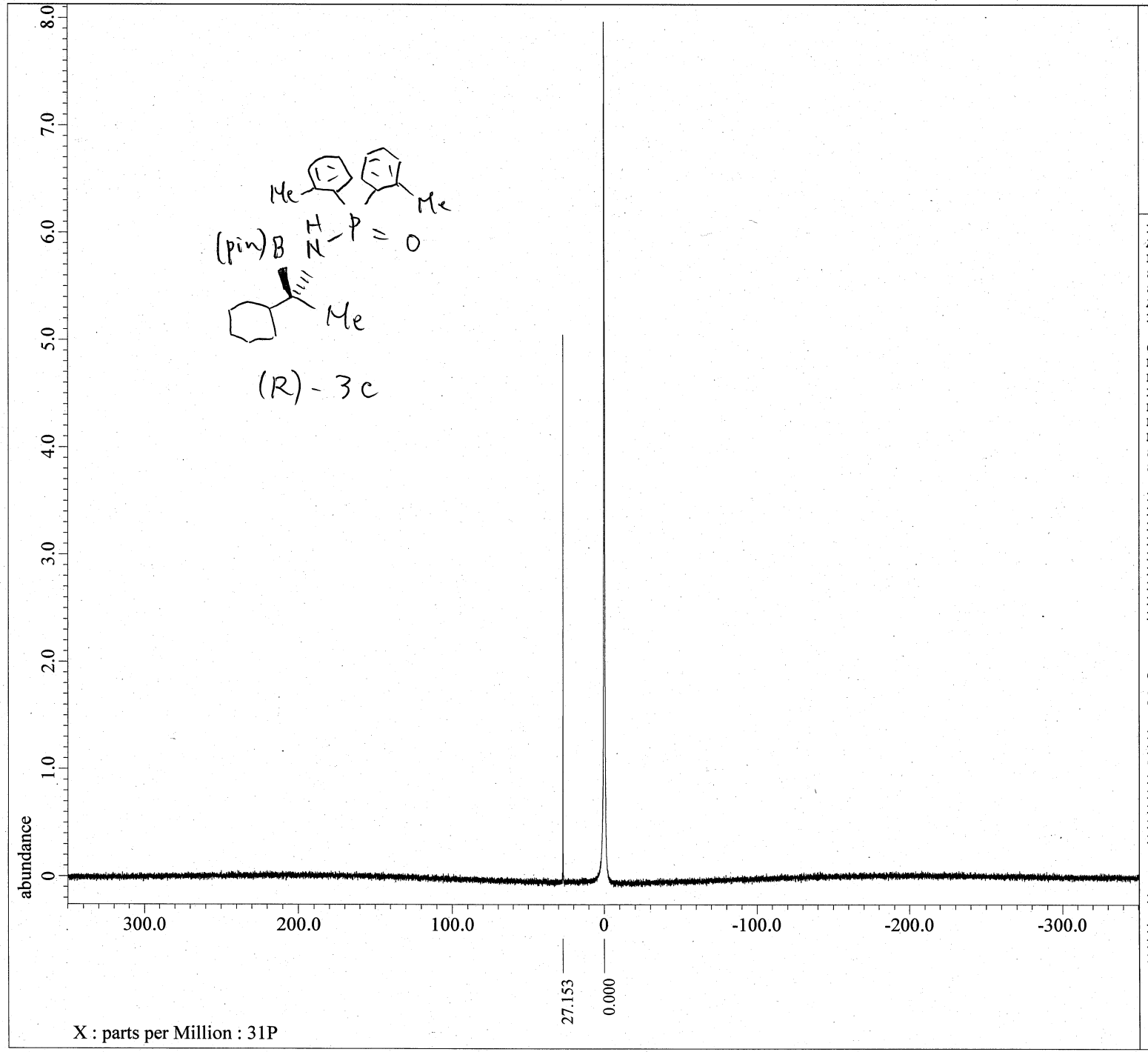
Filename	= MUR-145-proton-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#689386
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-OCT-2020 03:20:36
Revision_Time	= 31-JAN-2021 18:00:09
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 2.20725248[s]
X_Domain	= 1H
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 30
Temp_Get	= 19.2[dC]
X_90_Width	= 12.6[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 6.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.20725248[s]


abundance
X : parts per Million : 13C
(R)-3c
---- 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: MUR-145-13C-1.jdf
Filename = MUR-145-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-DEC-2020 02:43:28
Revision_Time = 31-JAN-2021 18:07:02
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 300
Total_Scans = 300
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 18.8[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]



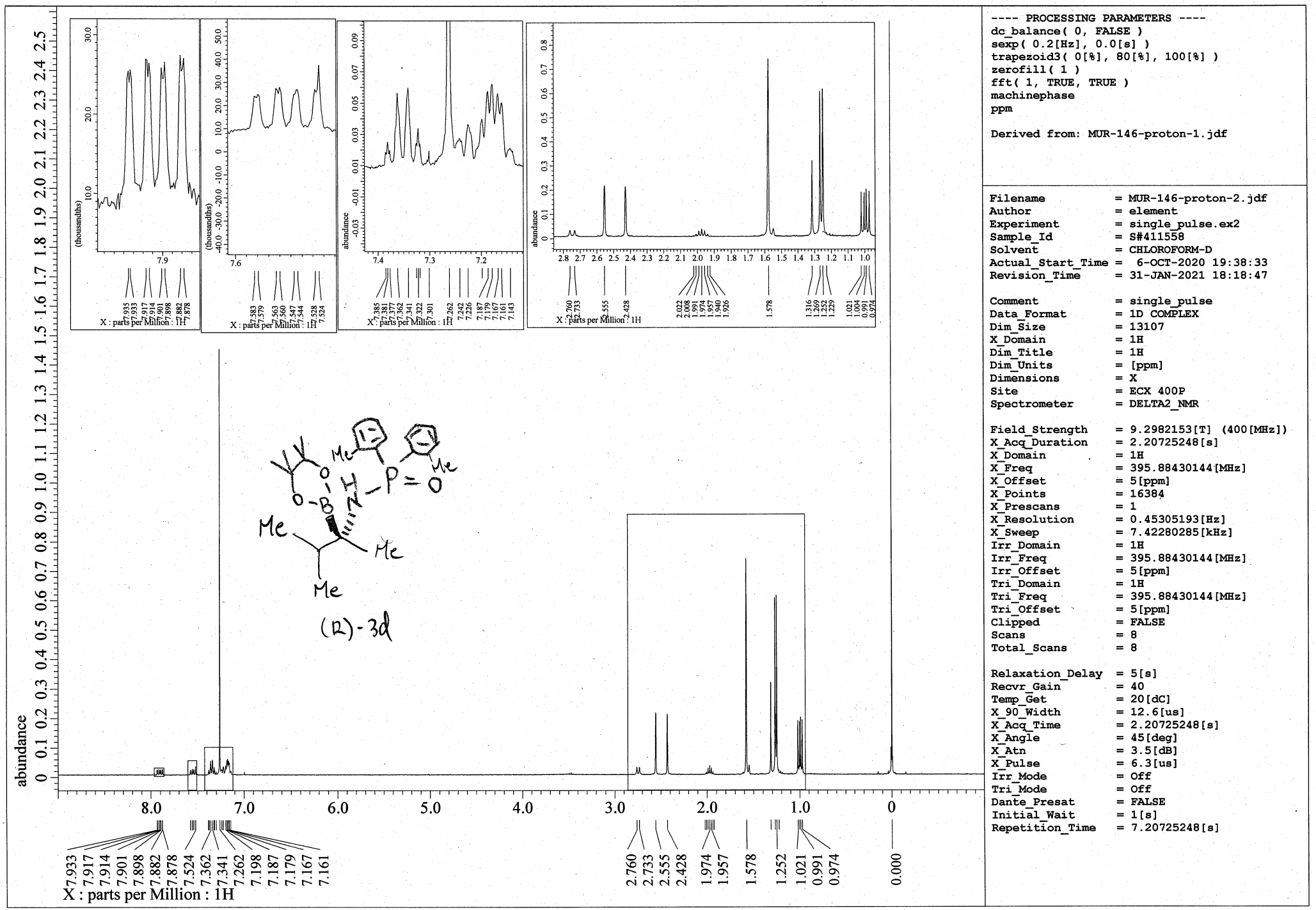

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-145-11B-1.jdf
```

```
Filename            = MUR-145-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#347712
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  2-MAR-2021 17:47:29
Revision_Time       =  4-MAR-2021 15:27:05

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 1000
Total_Scans         = 1000

Relaxation_Delay    = 2[s]
Recvr_Gain          = 48
Temp_Get            = 19.3[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```



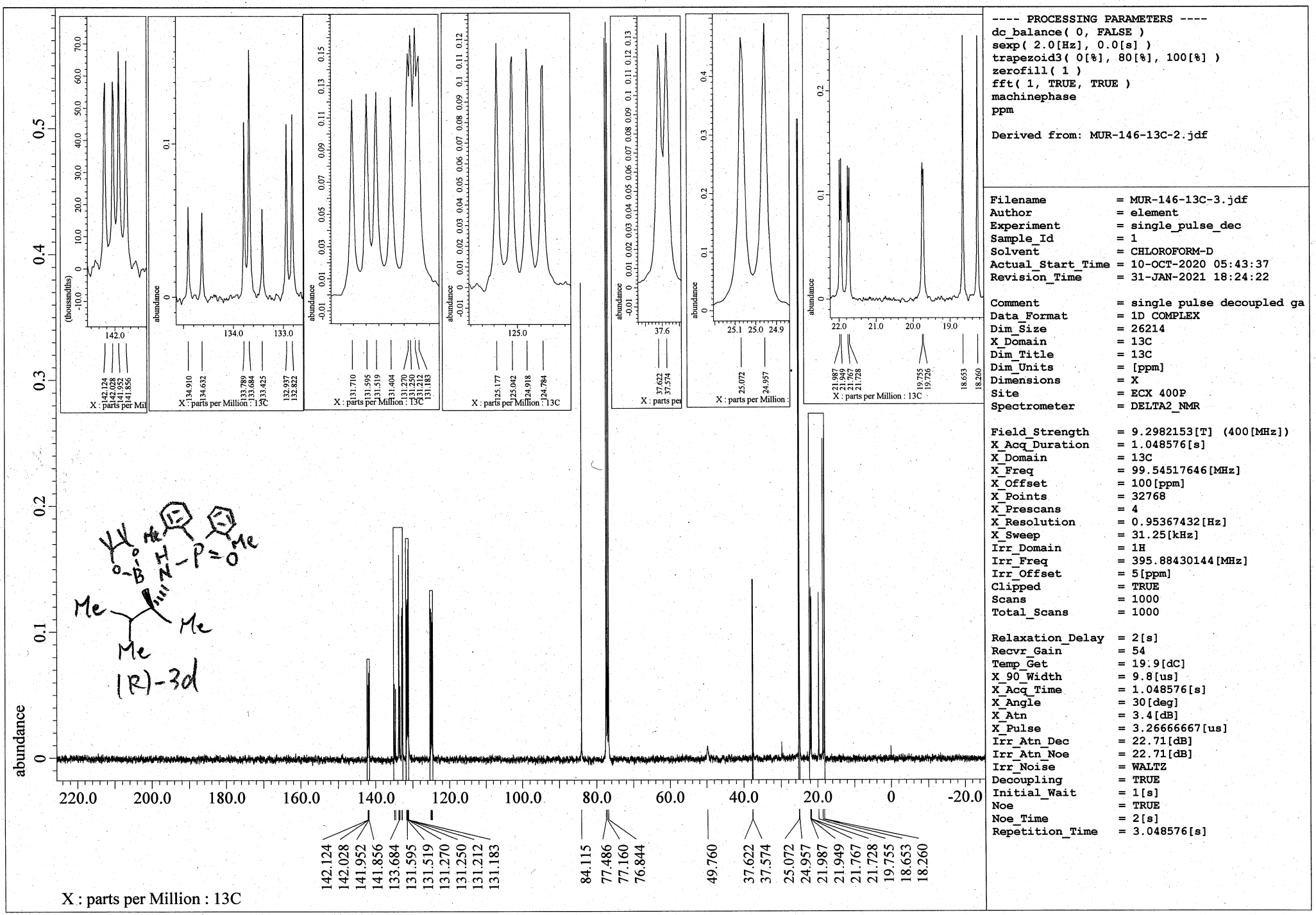

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-145-31P-1.jdf
```

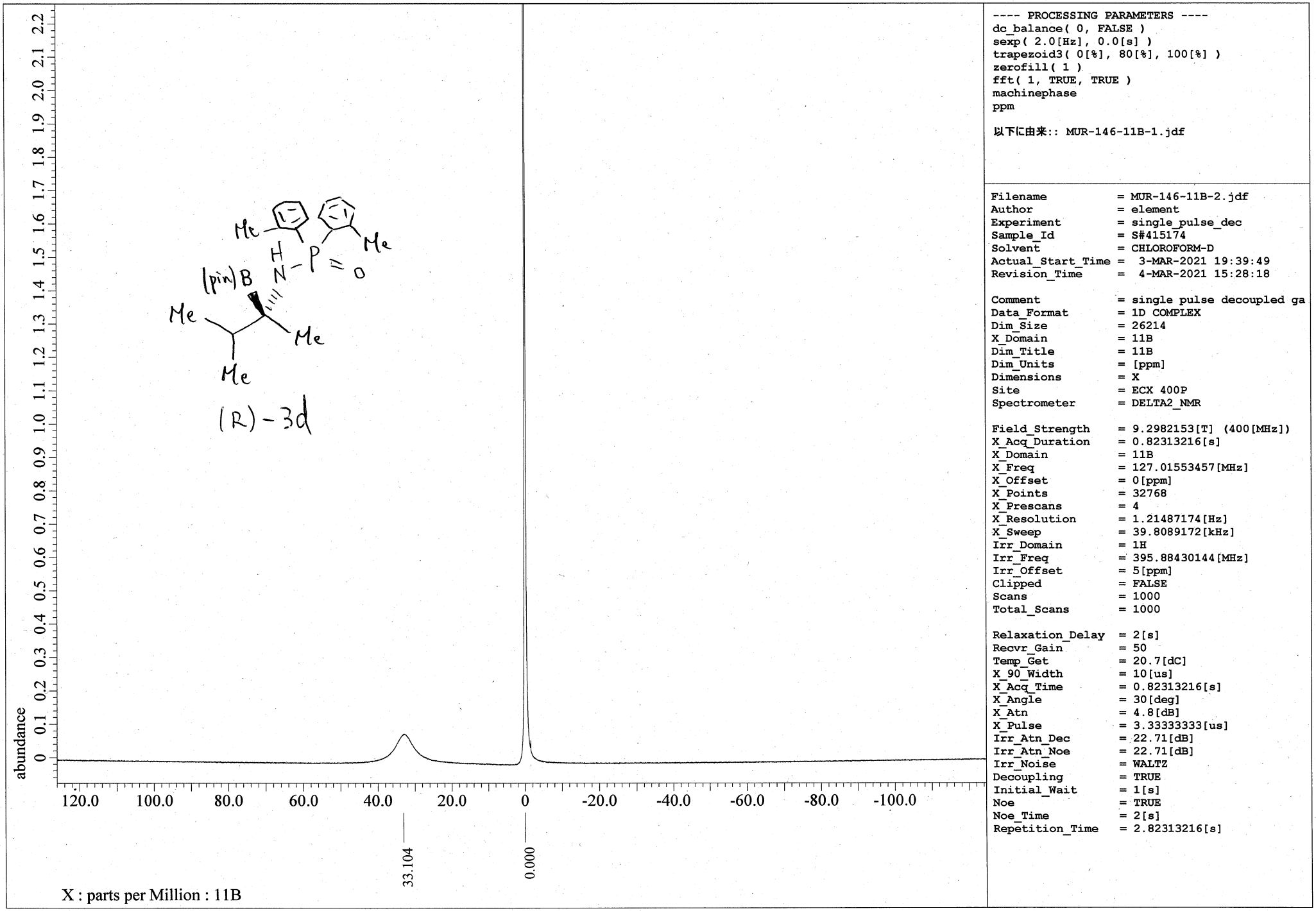
```
Filename            = MUR-145-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#420914
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 18:27:22
Revision_Time       =  6-MAY-2021 21:26:42

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 50
Total_Scans         = 50

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[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

Derived from: MUR-146-proton-1.jdf
```

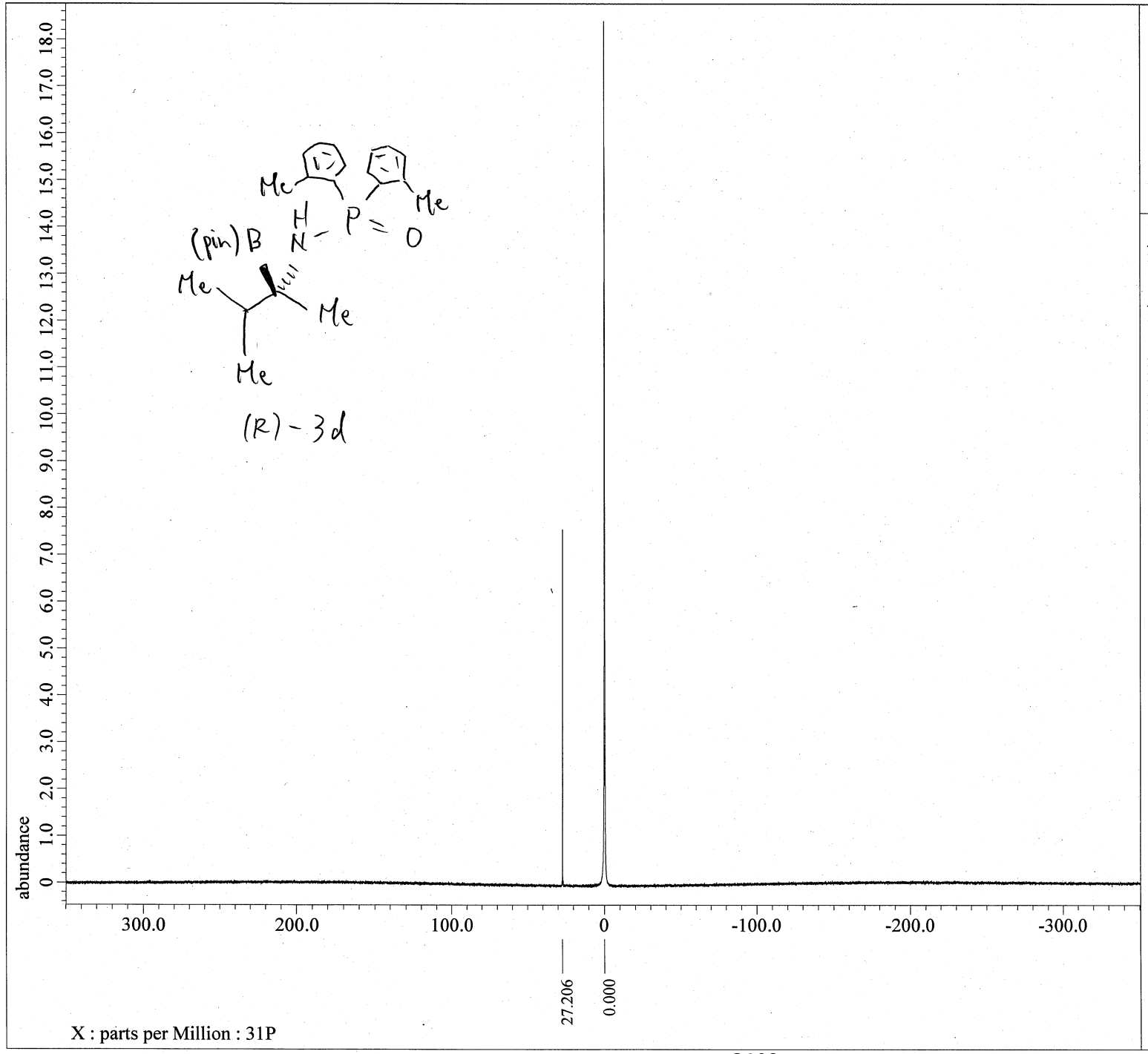
Filename	= MUR-146-proton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#411558
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-OCT-2020 19:38:33
Revision_Time	= 31-JAN-2021 18:18:47
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 2.20725248[s]
X_Domain	= 1H
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 20[dC]
X_90_Width	= 12.6[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 6.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.20725248[s]


abundance
X : parts per Million : 13C
(R)-3d
---- 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: MUR-146-13C-2.jdf
Filename = MUR-146-13C-3.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-OCT-2020 05:43:37
Revision_Time = 31-JAN-2021 18:24:22
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 19.9[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[s]



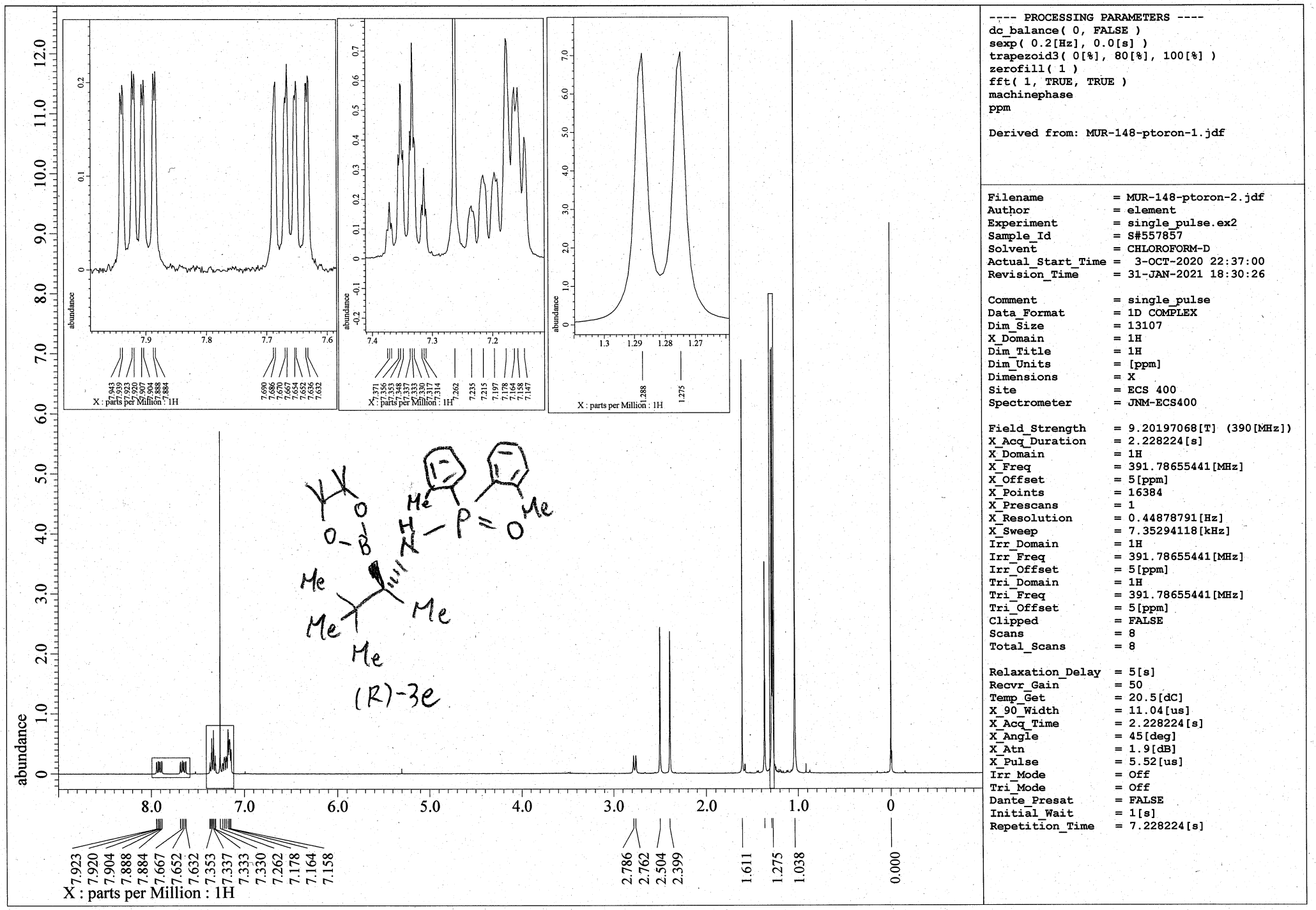

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-146-11B-1.jdf
```

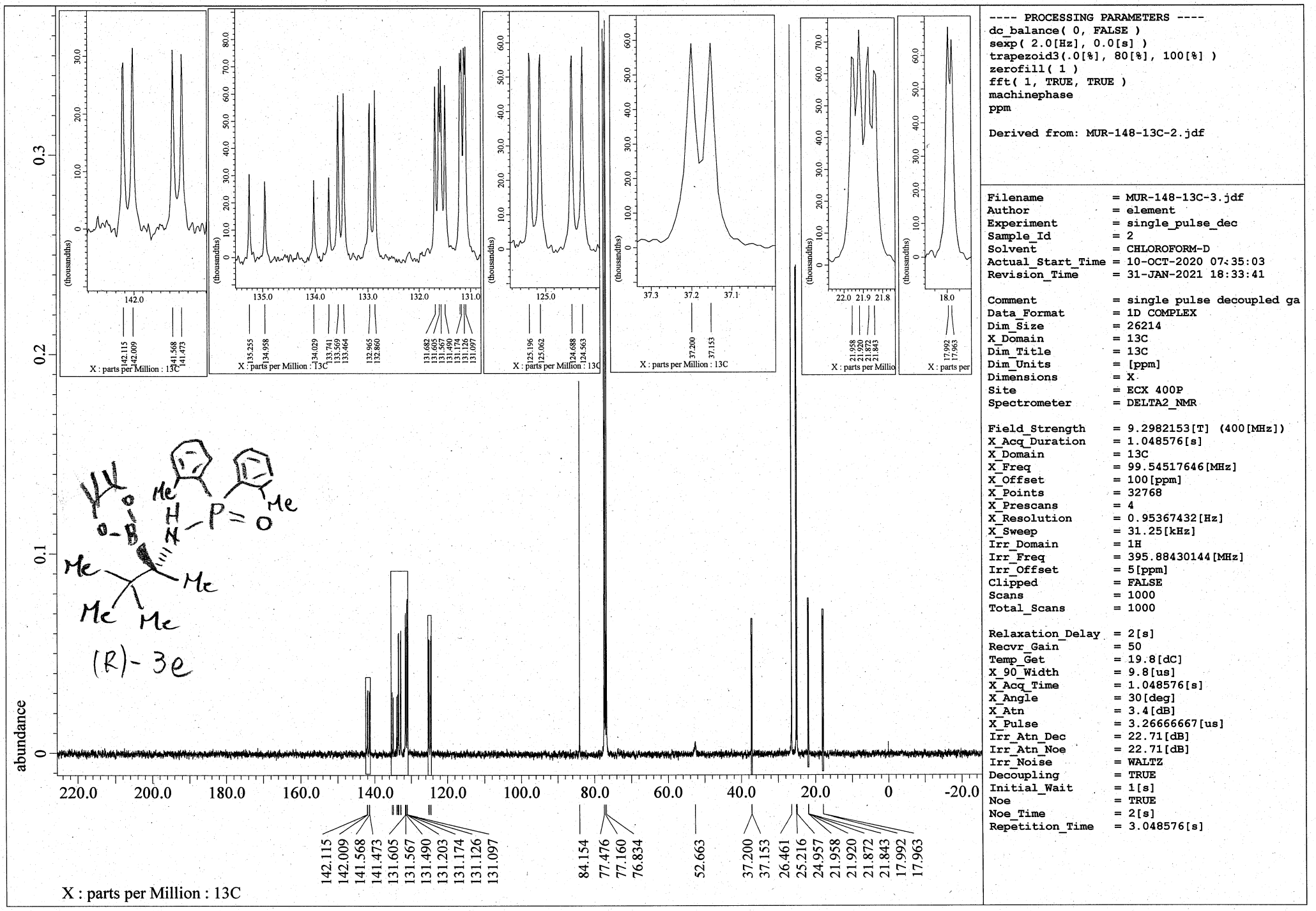
Filename	= MUR-146-11B-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#415174
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-MAR-2021 19:39:49
Revision_Time	= 4-MAR-2021 15:28:18
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 11B
Dim_Title	= 11B
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 0.82313216[s]
X_Domain	= 11B
X_Freq	= 127.01553457[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.21487174[Hz]
X_Sweep	= 39.8089172[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1000
Total_Scans	= 1000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.7[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 0.82313216[s]
X_Angle	= 30[deg]
X_Atn	= 4.8[dB]
X_Pulse	= 3.33333333[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Atn_Noe	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.82313216[s]

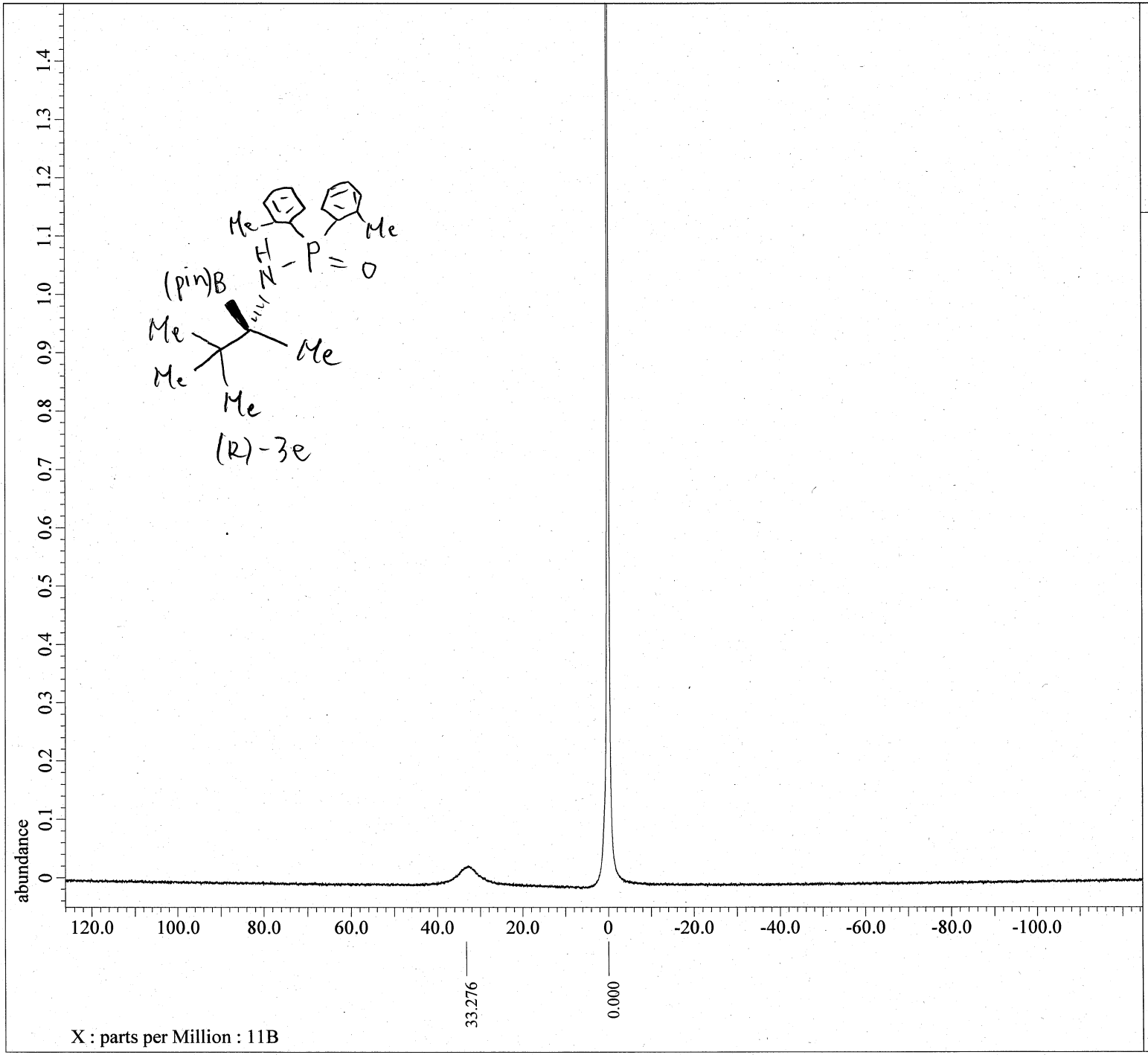



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-146-31P-1.jdf
```

```
Filename            = MUR-146-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#430408
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 18:43:10
Revision_Time       =  6-MAY-2021 21:27:12

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 50
Total_Scans         = 50

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```

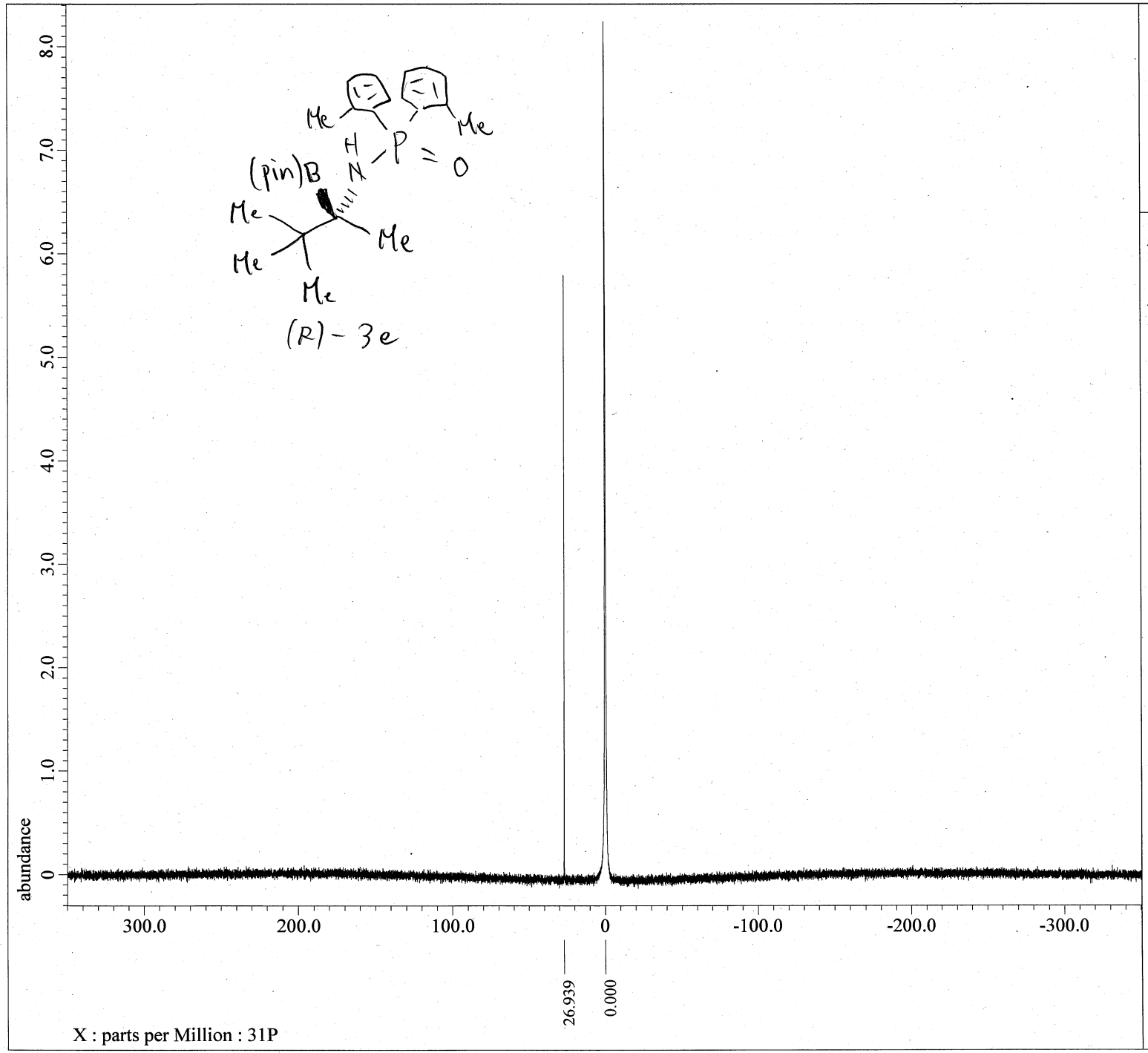

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-148-ptoron-1.jdf
Filename = MUR-148-ptoron-2.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#557857
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-OCT-2020 22:37:00
Revision_Time = 31-JAN-2021 18:30:26
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 2.228224[s]
X_Domain = 1H
X_Freq = 391.78655441[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.44878791[Hz]
X_Sweep = 7.35294118[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 391.78655441[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 20.5[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]
abundance
X : parts per Million : 1H
7.923 7.920 7.904 7.888 7.884 7.667 7.652 7.632 7.353 7.337 7.333 7.330 7.262 7.178 7.164 7.158
2.786 2.762 2.504 2.399 1.611 1.275 1.038 0.000
Me
Me
Me
Me
Me
(R)-3e


---- 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: MUR-148-13C-2.jdf
Filename = MUR-148-13C-3.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 2
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-OCT-2020 07:35:03
Revision_Time = 31-JAN-2021 18:33:41
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.8[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[s]
(thousandths)
abundance
0
0.1
0.2
0.3
220.0
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0
-20.0
142.115
142.009
141.568
141.473
131.605
131.567
131.490
131.203
131.174
131.126
131.097
84.154
77.476
77.160
76.834
52.663
37.200
37.153
26.461
25.216
24.957
21.958
21.920
21.872
21.843
17.992
17.963
X : parts per Million : 13C
Me
H
N
P
O
Me
Me
Me
Me
(R)-3e



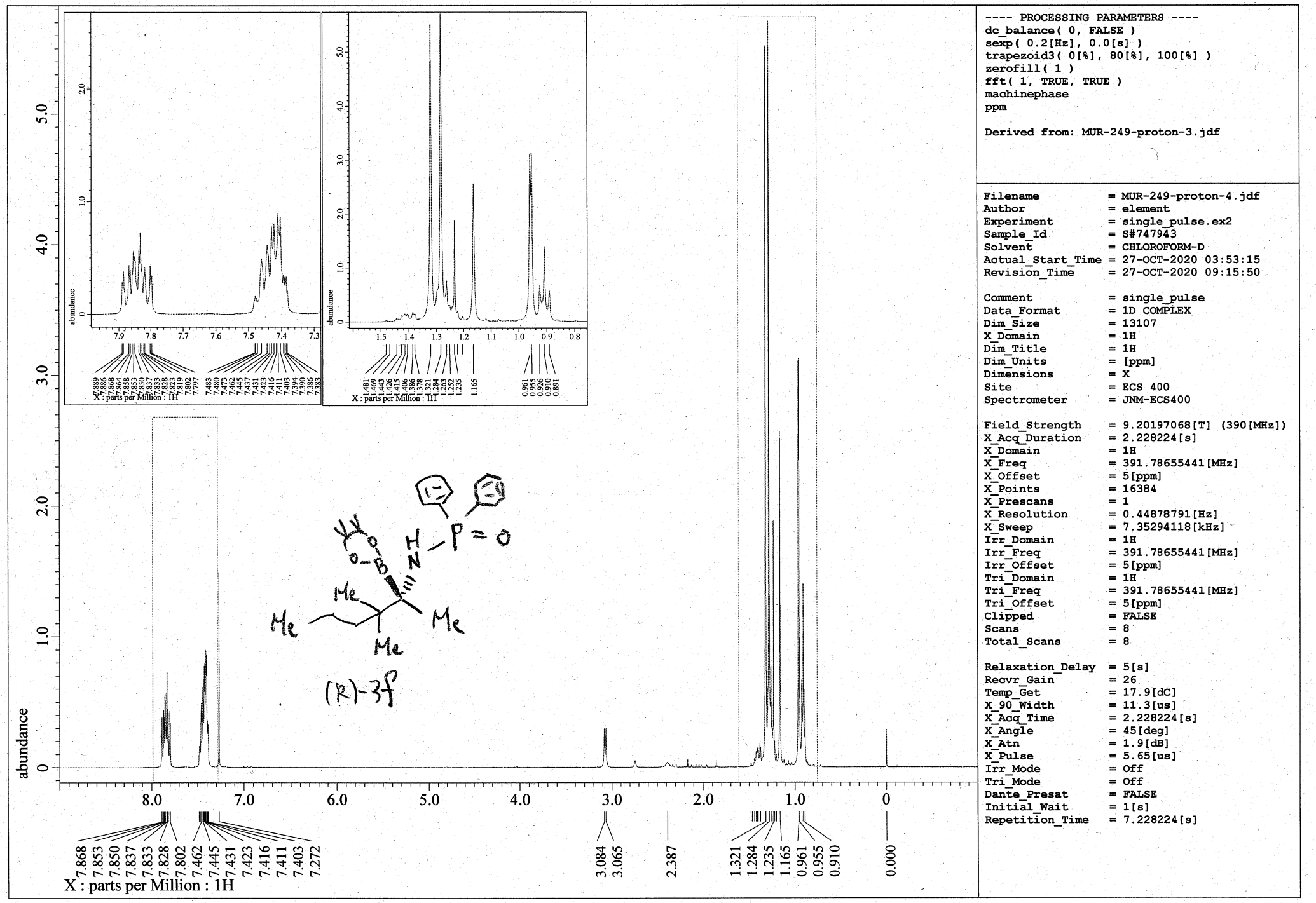

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-148-11B-1.jdf
```

```
Filename            = MUR-148-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#481771
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  3-MAR-2021 21:31:08
Revision_Time       =  4-MAR-2021 15:31:31

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 500
Total_Scans         = 500

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.3[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```



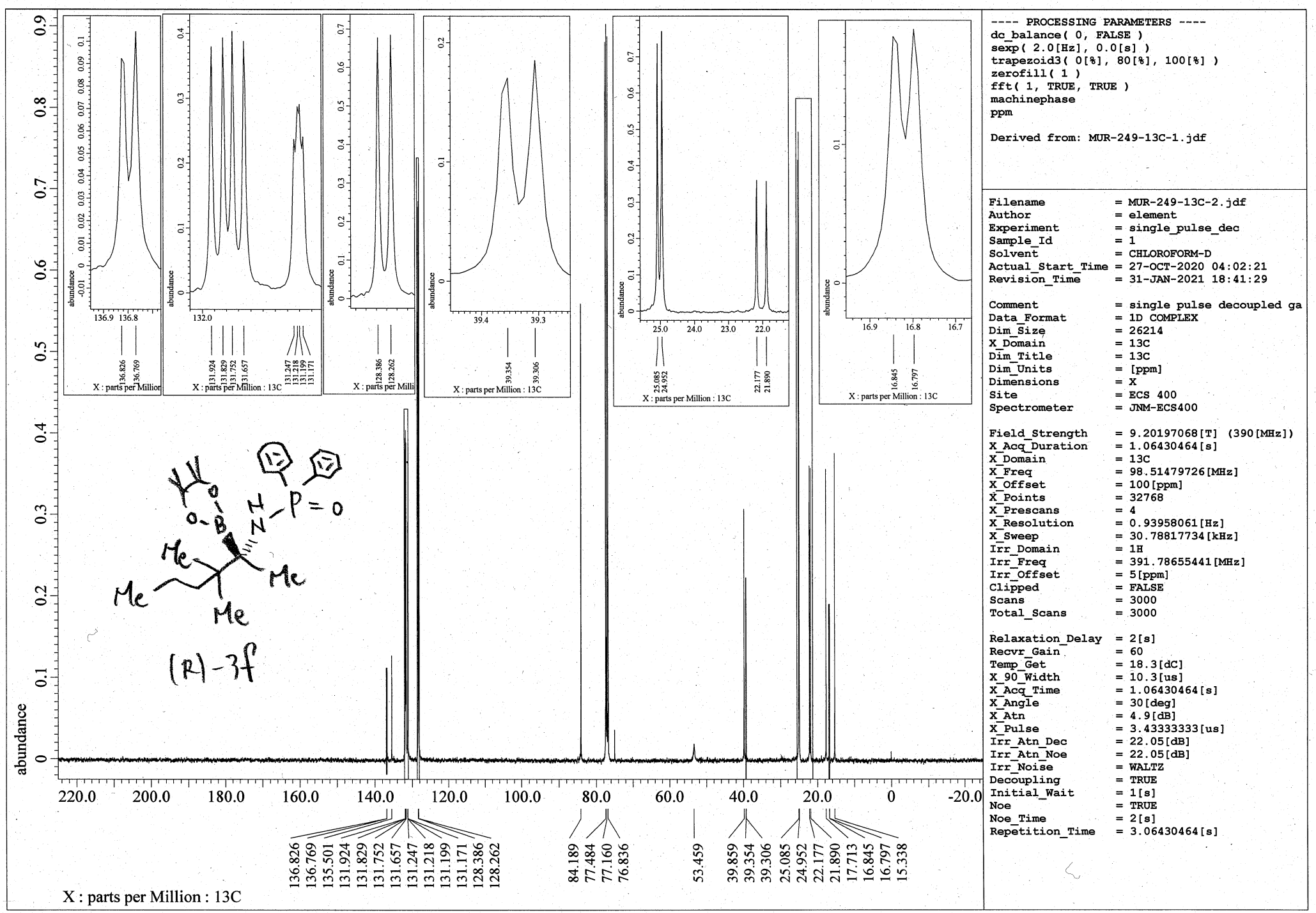

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-148-31P-1.jdf
```

```
Filename           = MUR-148-31P-2.jdf
Author             = element
Experiment         = single_pulse_dec
Sample_Id          = S#451353
Solvent            = CHLOROFORM-D
Actual_Start_Time  = 27-APR-2021 19:18:04
Revision_Time      =  6-MAY-2021 21:27:40

Comment            = single pulse decoupled ga
Data_Format        = 1D COMPLEX
Dim_Size           = 26214
X_Domain           = 31P
Dim_Title          = 31P
Dim_Units          = [ppm]
Dimensions         = X
Site               = ECS 400
Spectrometer       = JNM-ECS400

Field_Strength     = 9.20197068[T] (390[MHz])
X_Acq_Duration     = 0.2359296[s]
X_Domain           = 31P
X_Freq             = 158.59799923[MHz]
X_Offset           = 0[ppm]
X_Points           = 32768
X_Prescans         = 4
X_Resolution       = 4.23855252[Hz]
X_Sweep            = 138.88888889[kHz]
Irr_Domain         = 1H
Irr_Freq           = 391.78655441[MHz]
Irr_Offset         = 5[ppm]
Clipped            = FALSE
Scans              = 20
Total_Scans        = 20

Relaxation_Delay   = 2[s]
Recvr_Gain         = 50
Temp_Get           = 19.2[dC]
X_90_Width         = 12.25[us]
X_Acq_Time         = 0.2359296[s]
X_Angle            = 30[deg]
X_Atn              = 5.5[dB]
X_Pulse            = 4.08333333[us]
Irr_Atn_Dec        = 22.45[dB]
Irr_Atn_Noe        = 22.45[dB]
Irr_Noise          = WALTZ
Decoupling         = TRUE
Initial_Wait       = 1[s]
Noe                = TRUE
Noe_Time           = 2[s]
Repetition_Time    = 2.2359296[s]
```



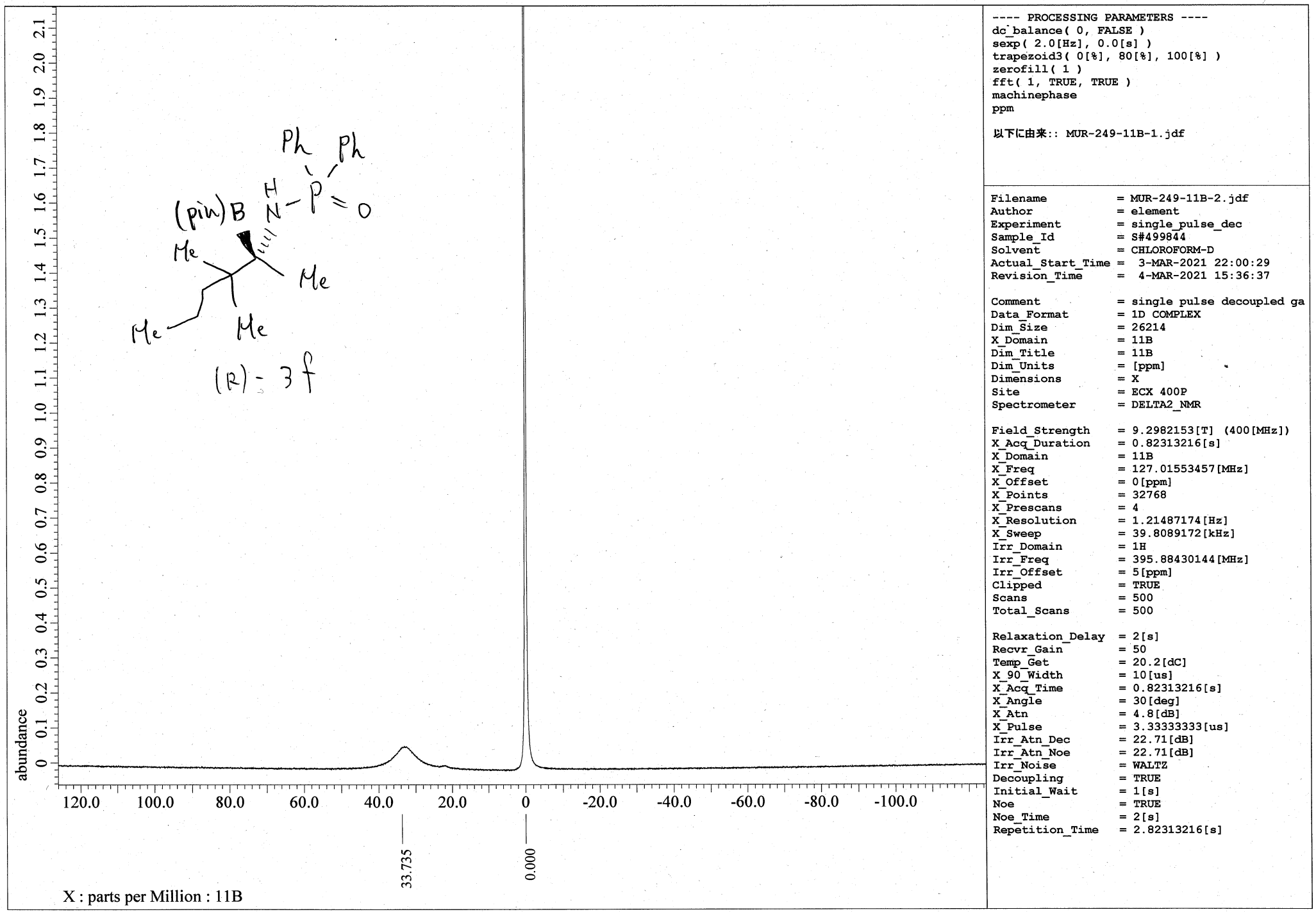

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-249-proton-3.jdf
```

Filename	= MUR-249-proton-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#747943
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-OCT-2020 03:53:15
Revision_Time	= 27-OCT-2020 09:15:50
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	= 26
Temp_Get	= 17.9[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]



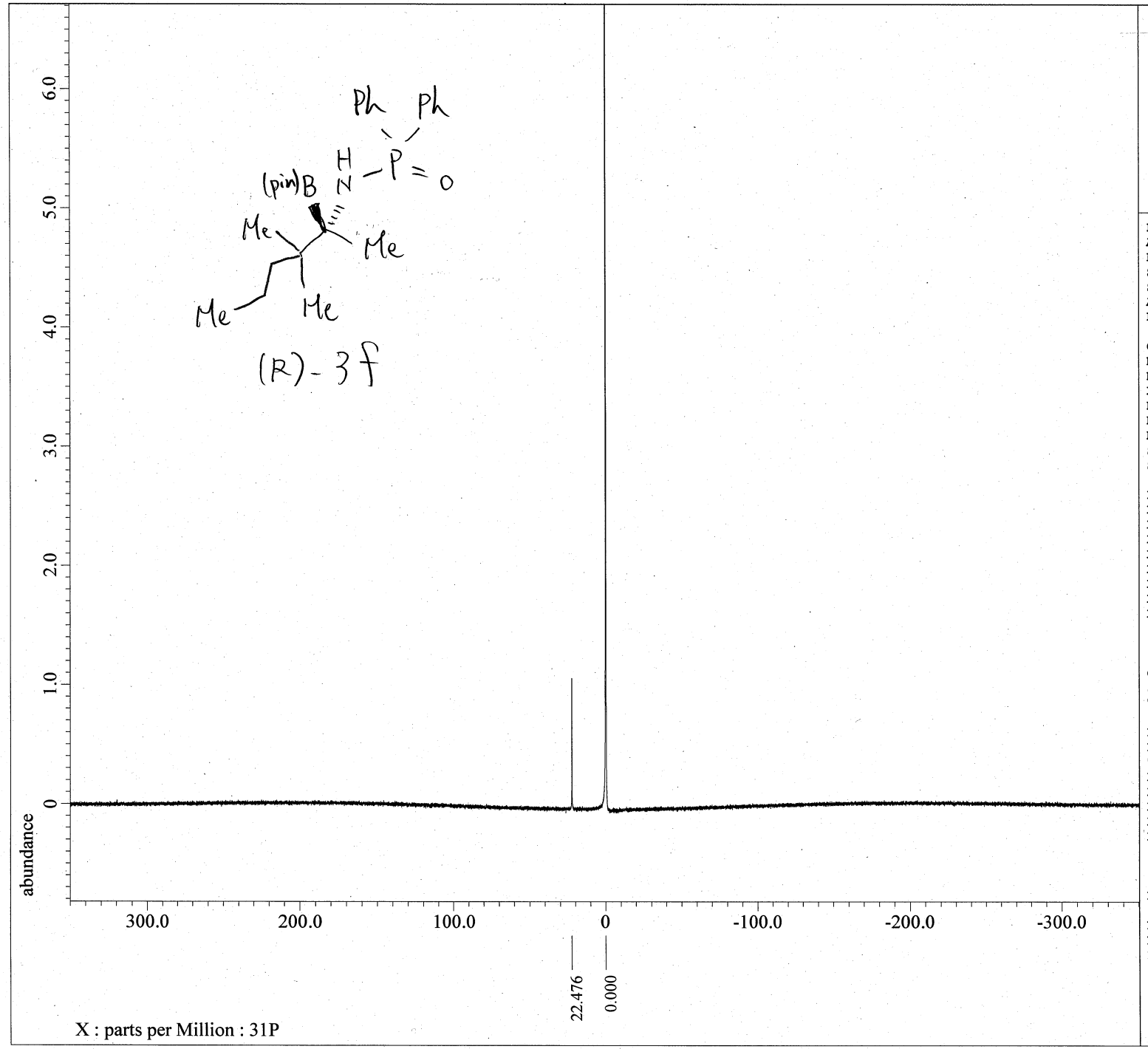

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-249-13C-1.jdf
```

Filename	= MUR-249-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-OCT-2020 04:02:21
Revision_Time	= 31-JAN-2021 18:41:29
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 3000
Total_Scans	= 3000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.3[dC]
X_90_Width	= 10.3[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.43333333[us]
Irr_Atn_Dec	= 22.05[dB]
Irr_Atn_Noe	= 22.05[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



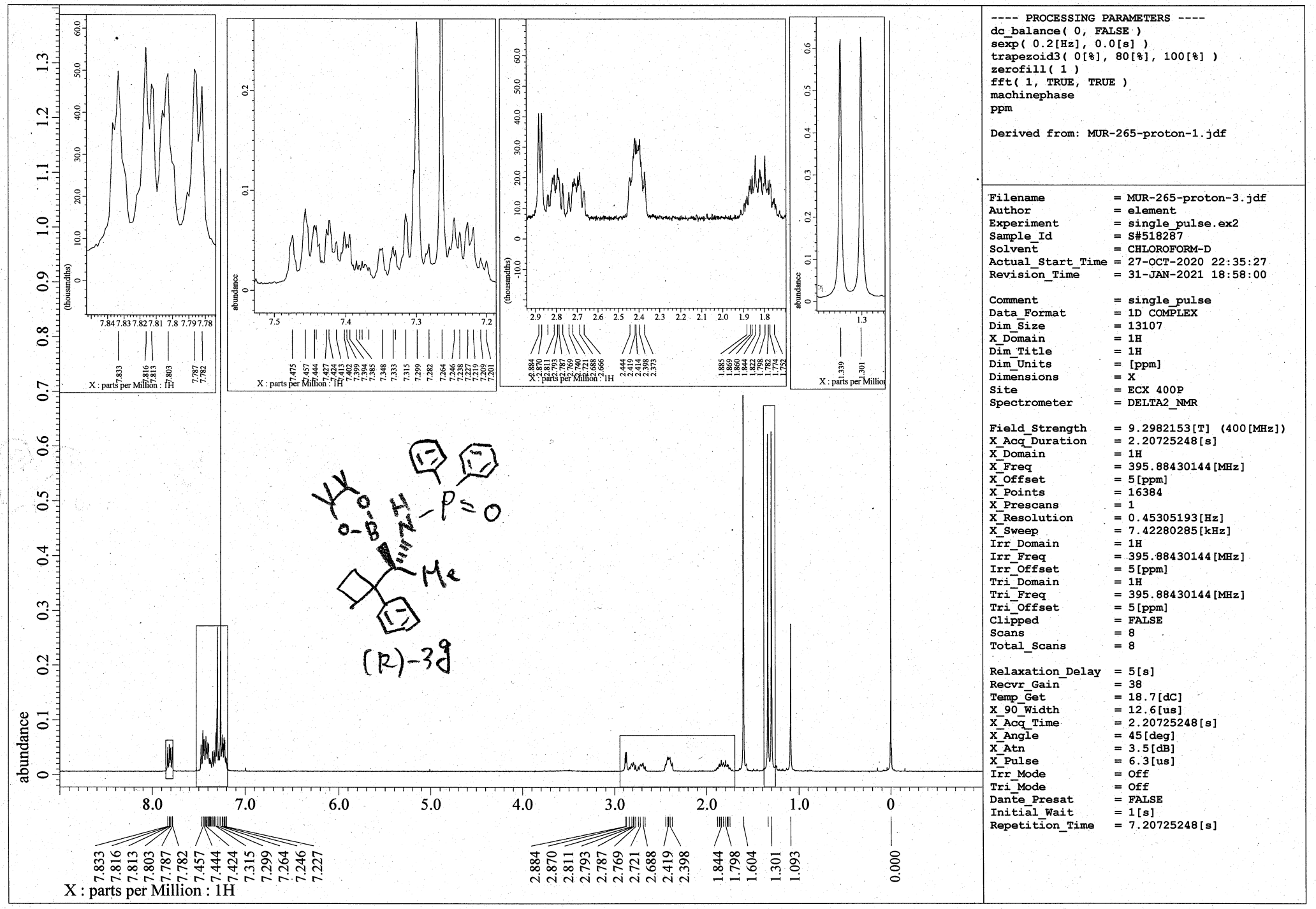

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-249-11B-1.jdf
```

```
Filename            = MUR-249-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#499844
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  3-MAR-2021 22:00:29
Revision_Time       =  4-MAR-2021 15:36:37

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = TRUE
Scans               = 500
Total_Scans         = 500

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20.2[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```



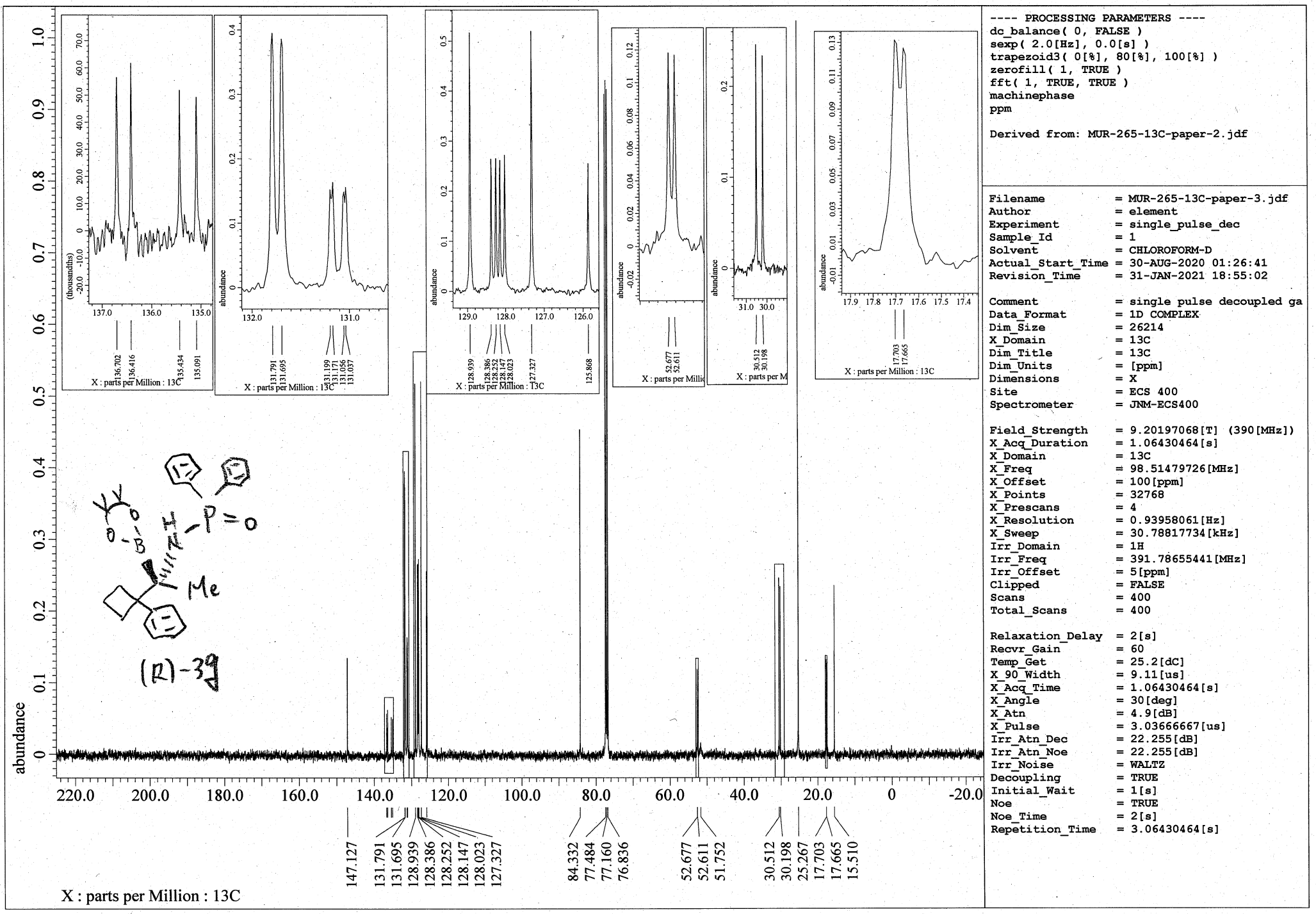

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-249-31P-1.jdf
```

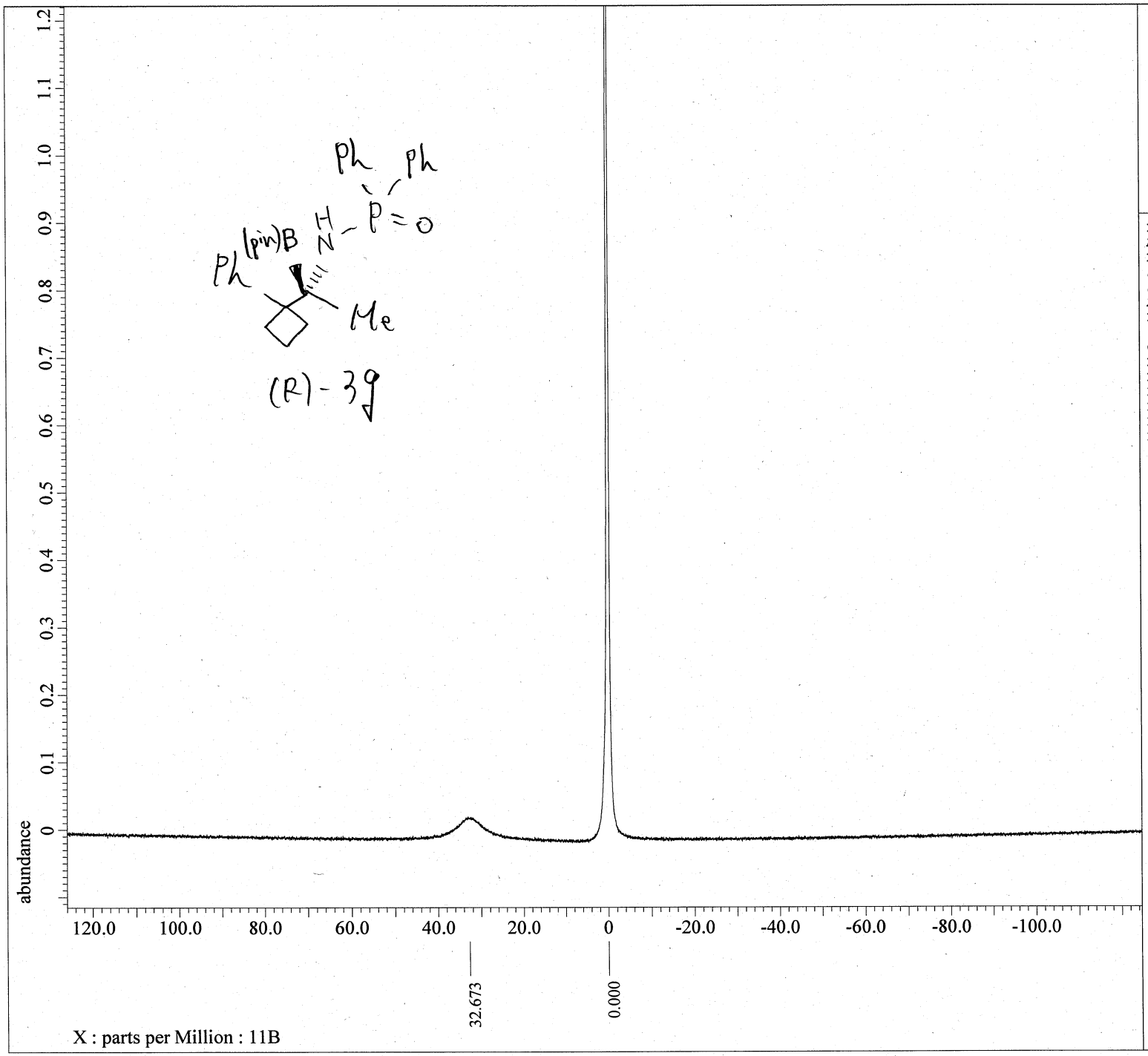
```
Filename            = MUR-249-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#455748
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 19:25:28
Revision_Time       =  6-MAY-2021 21:35:50

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[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          = 48
Temp_Get            = 18.8[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[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

Derived from: MUR-265-proton-1.jdf
```

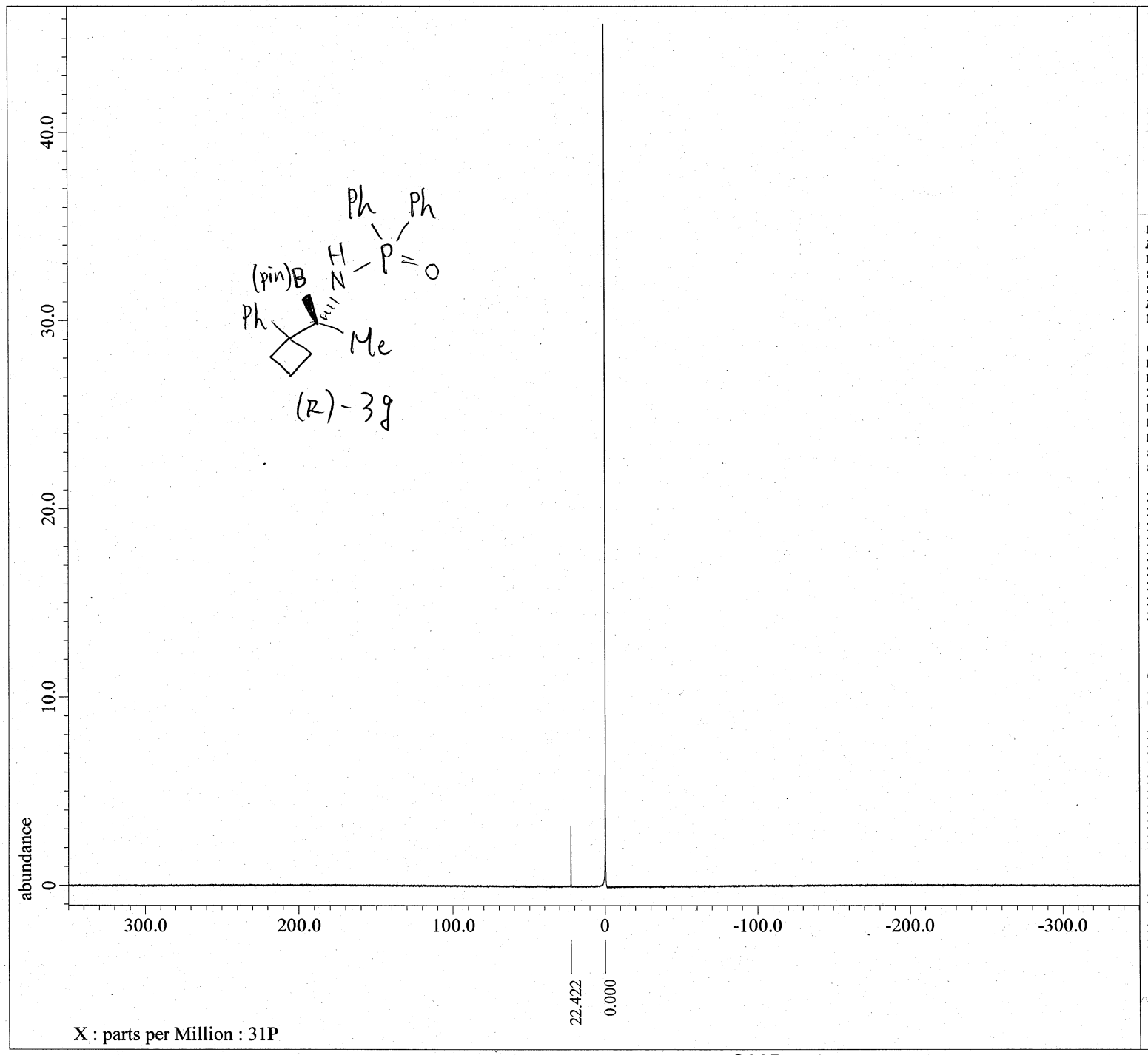
Filename	= MUR-265-proton-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#518287
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-OCT-2020 22:35:27
Revision_Time	= 31-JAN-2021 18:58:00
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 2.20725248[s]
X_Domain	= 1H
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 38
Temp_Get	= 18.7[dC]
X_90_Width	= 12.6[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 6.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.20725248[s]


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-265-13C-paper-2.jdf
Filename = MUR-265-13C-paper-3.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-AUG-2020 01:26:41
Revision_Time = 31-JAN-2021 18:55:02
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 400
Total_Scans = 400
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25.2[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]
abundance
X : parts per Million : 13C
147.127
131.791
131.695
128.939
128.386
128.252
128.147
128.023
127.327
84.332
77.484
77.160
76.836
52.677
52.611
51.752
30.512
30.198
25.267
17.703
17.665
15.510
Me
(R)-39



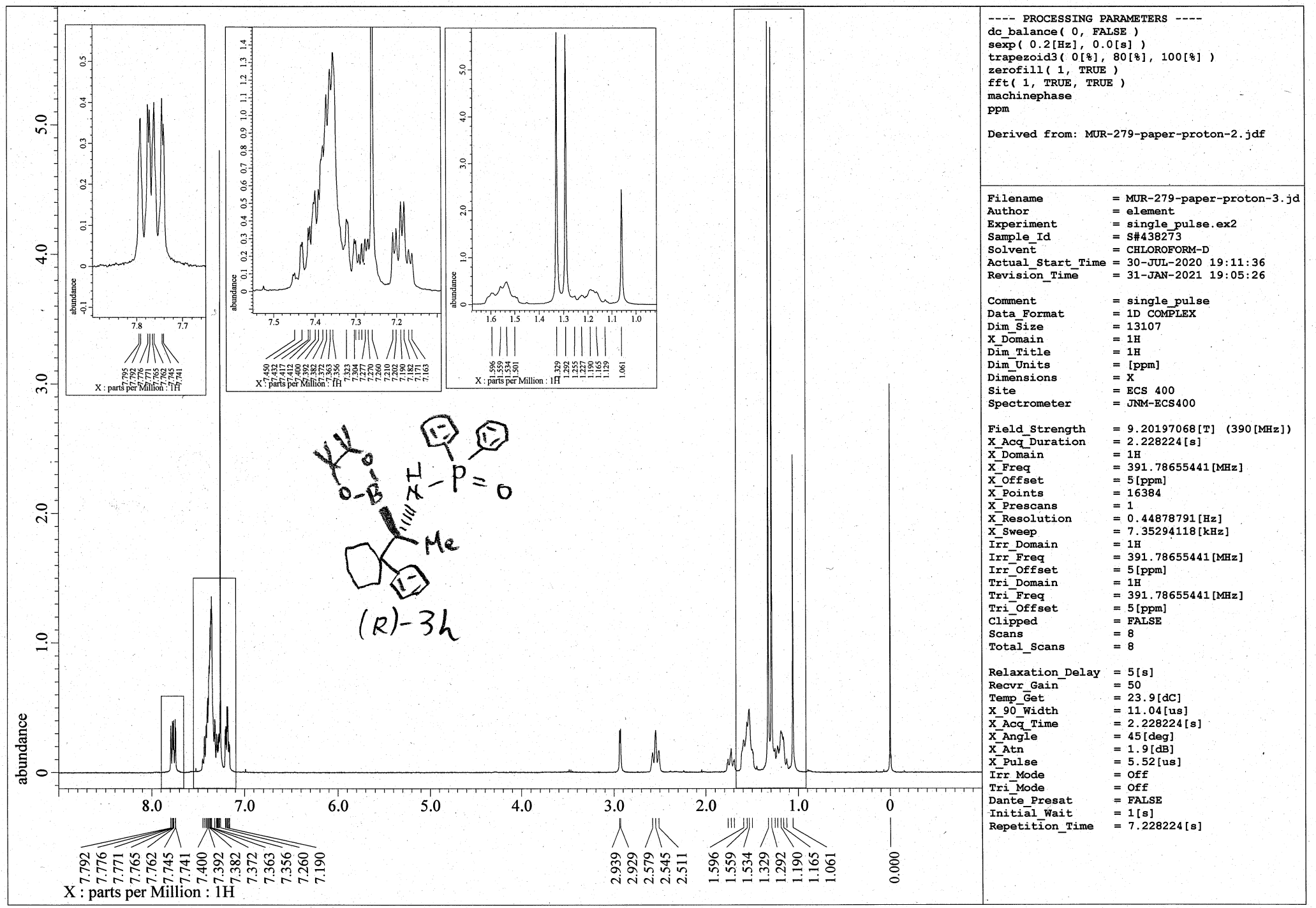

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-265-11B-1.jdf
```

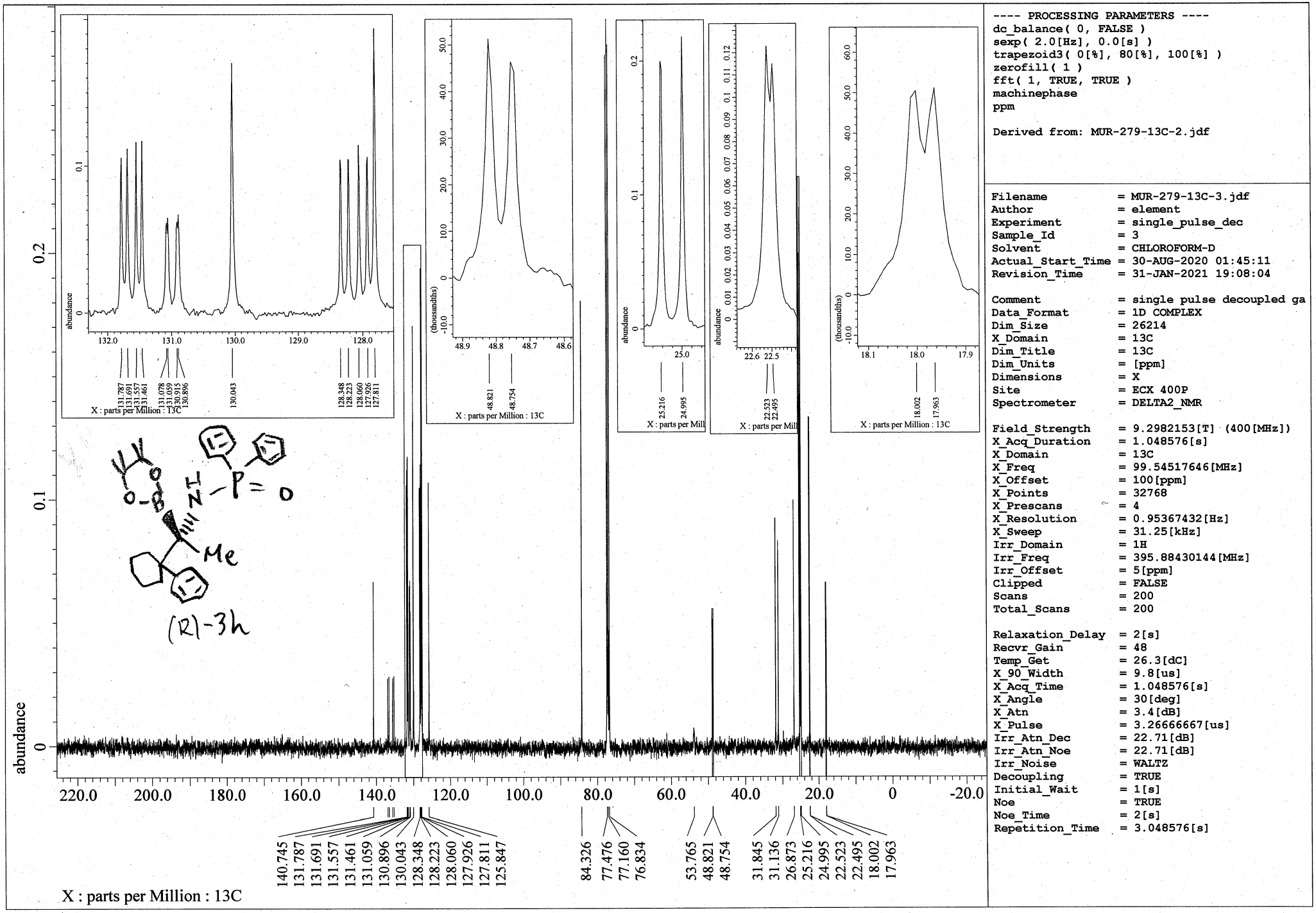
```
Filename            = MUR-265-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#535976
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  3-MAR-2021 23:01:02
Revision_Time       =  4-MAR-2021 15:23:28

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 500
Total_Scans         = 500

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.8[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```

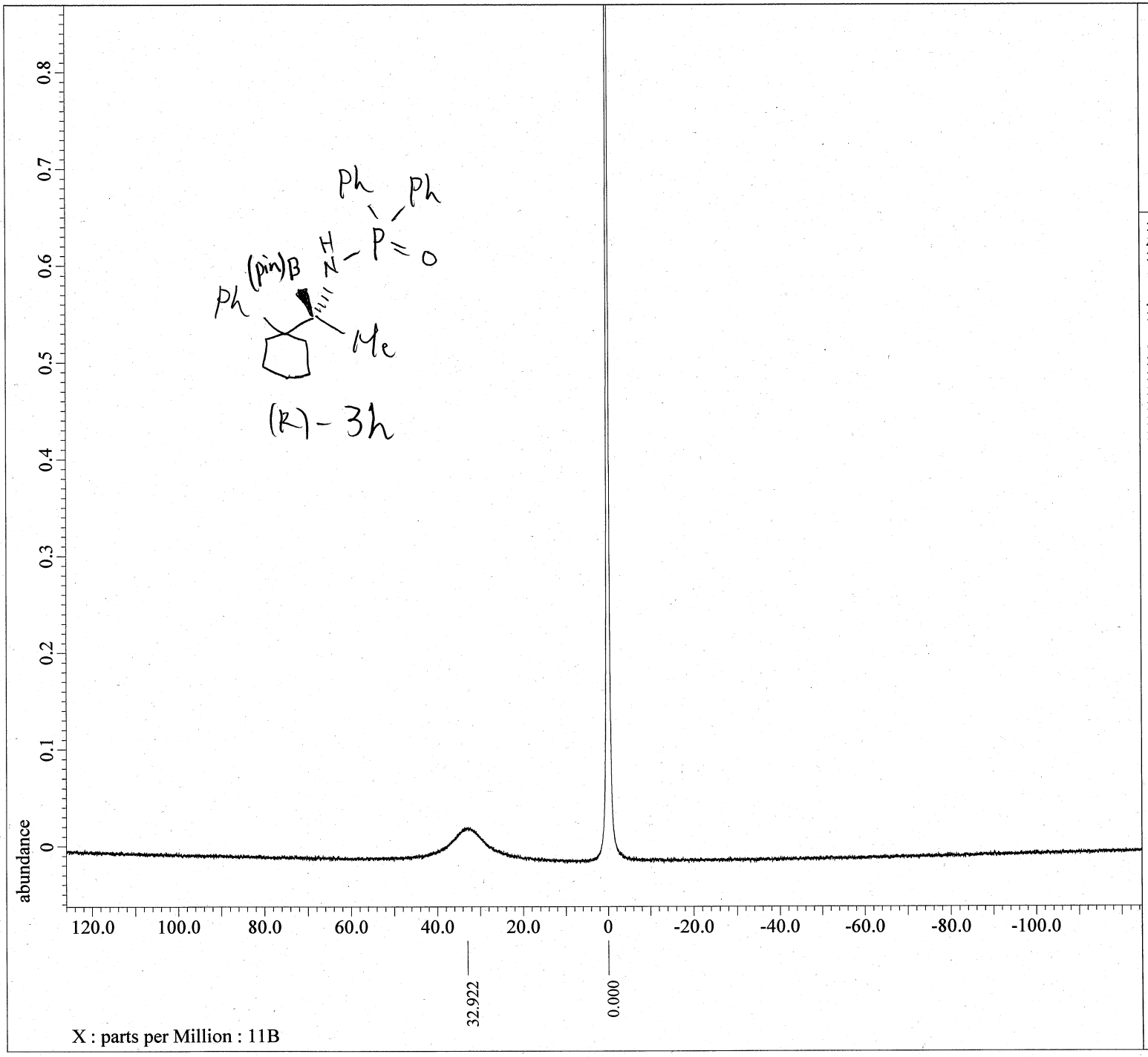



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-265-31P-1.jdf
```

```
Filename            = MUR-265-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#480810
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 20:08:08
Revision_Time       =  6-MAY-2021 21:25:44

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```

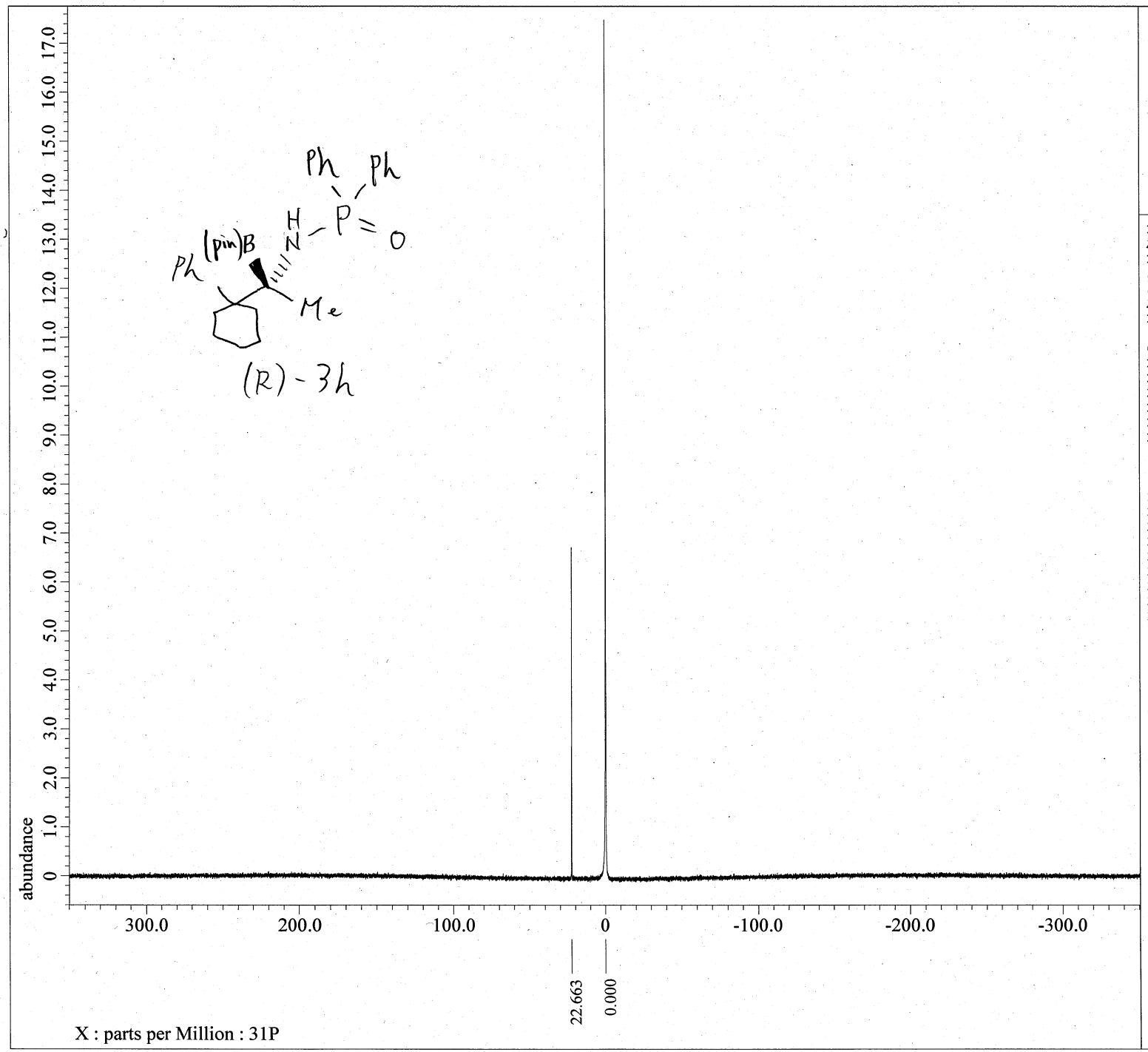

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-279-paper-proton-2.jdf
Filename = MUR-279-paper-proton-3.jd
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#438273
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-JUL-2020 19:11:36
Revision_Time = 31-JAN-2021 19:05:26
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 2.228224[s]
X_Domain = 1H
X_Freq = 391.78655441[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.44878791[Hz]
X_Sweep = 7.35294118[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 391.78655441[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 23.9[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]
abundance
X : parts per Million : 1H
7.792 7.776 7.771 7.765 7.762 7.745 7.741 7.400 7.392 7.382 7.372 7.363 7.356 7.260 7.190
2.939 2.929 2.579 2.545 2.511
1.596 1.559 1.534 1.329 1.292 1.190 1.165 1.061
0.000
Me
(R)-3h


---- 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: MUR-279-13C-2.jdf
Filename = MUR-279-13C-3.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 3
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-AUG-2020 01:45:11
Revision_Time = 31-JAN-2021 19:08:04
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 26.3[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[s]
abundance
X : parts per Million : 13C
(R)-3h
Me
140.745
131.787
131.691
131.557
131.461
131.059
130.896
130.043
128.348
128.223
128.060
127.926
127.811
125.847
84.326
77.476
77.160
76.834
53.765
48.821
48.754
31.845
31.136
26.873
25.216
24.995
22.523
22.495
18.002
17.963



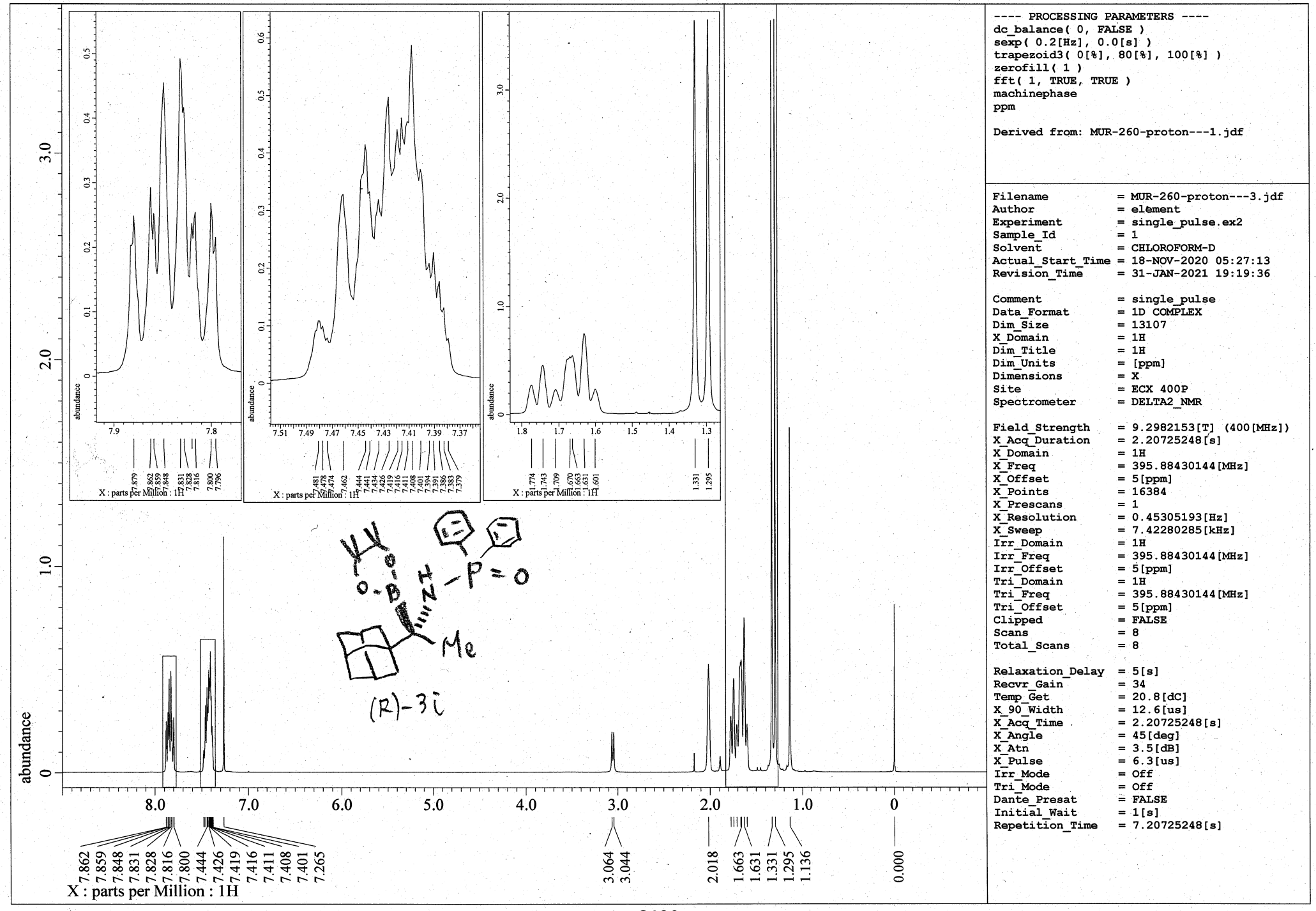

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-279-11B-1.jdf
```

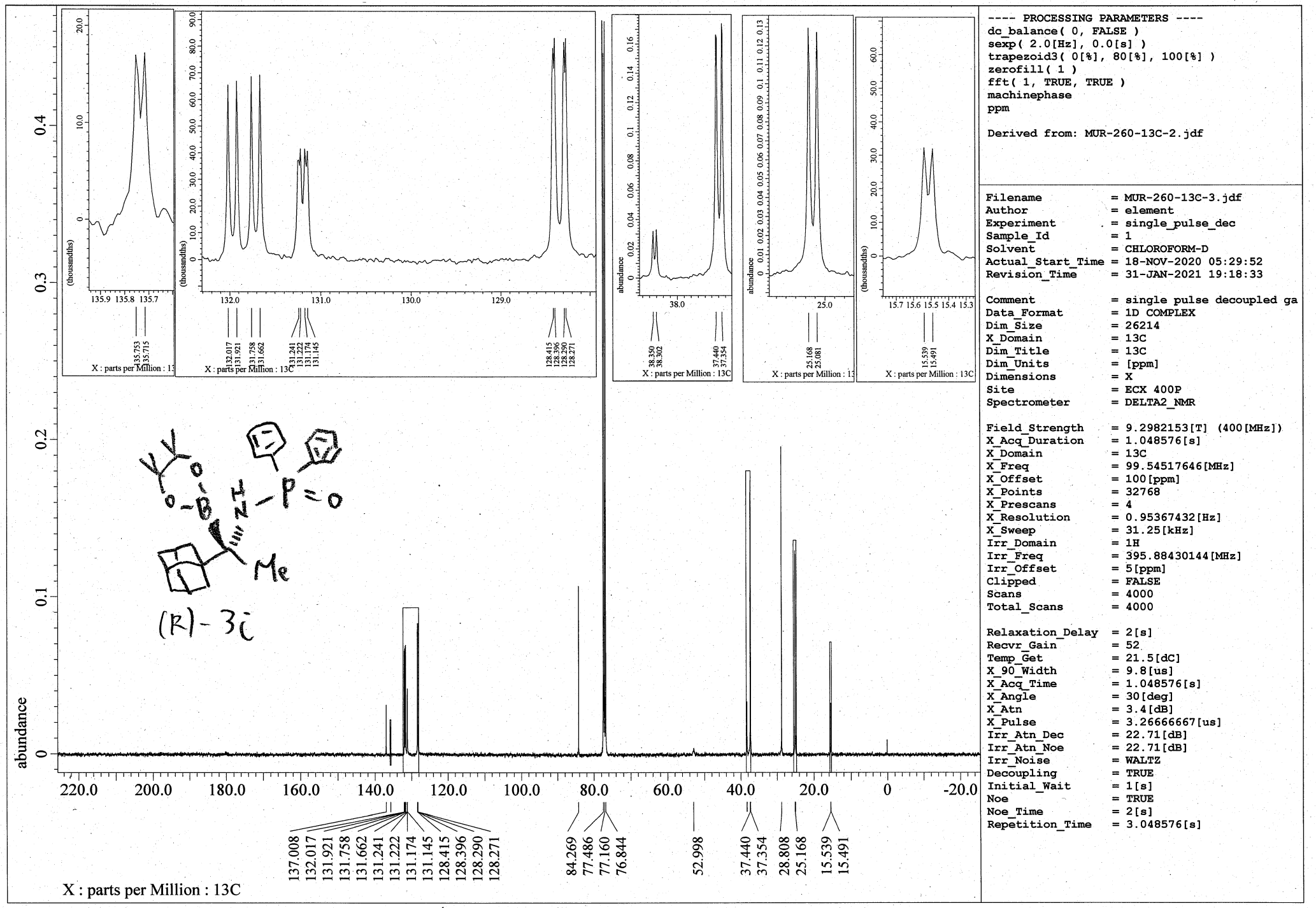
```
Filename            = MUR-279-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#588057
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  4-MAR-2021 00:27:35
Revision_Time       =  4-MAR-2021 15:24:35

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 455
Total_Scans         = 455

Relaxation_Delay    = 2[s]
Recvr_Gain          = 48
Temp_Get            = 20[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```

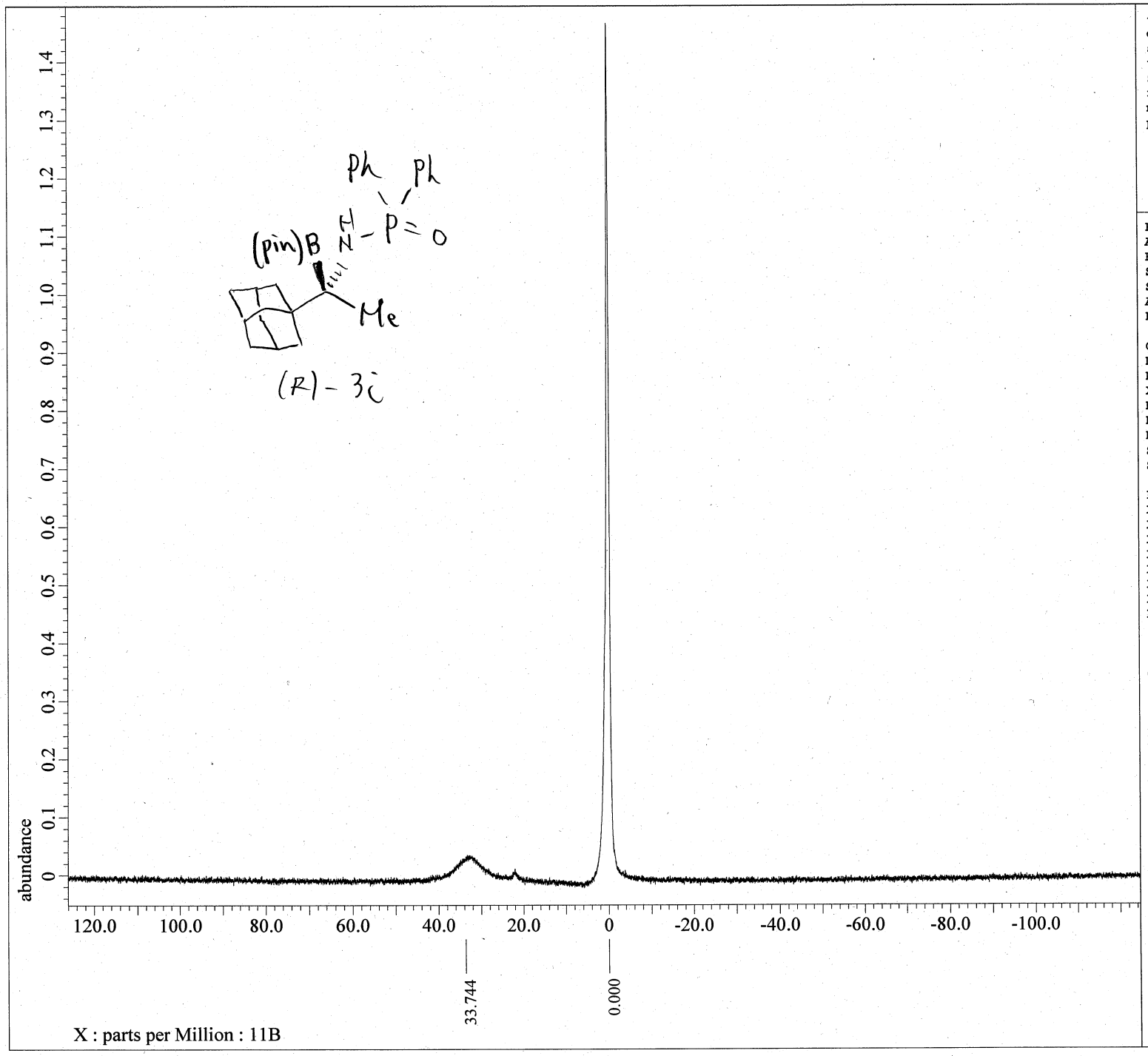



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-279-31P-1.jdf
```

```
Filename            = MUR-279-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#484563
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 20:13:25
Revision_Time       =  6-MAY-2021 21:37:13

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```

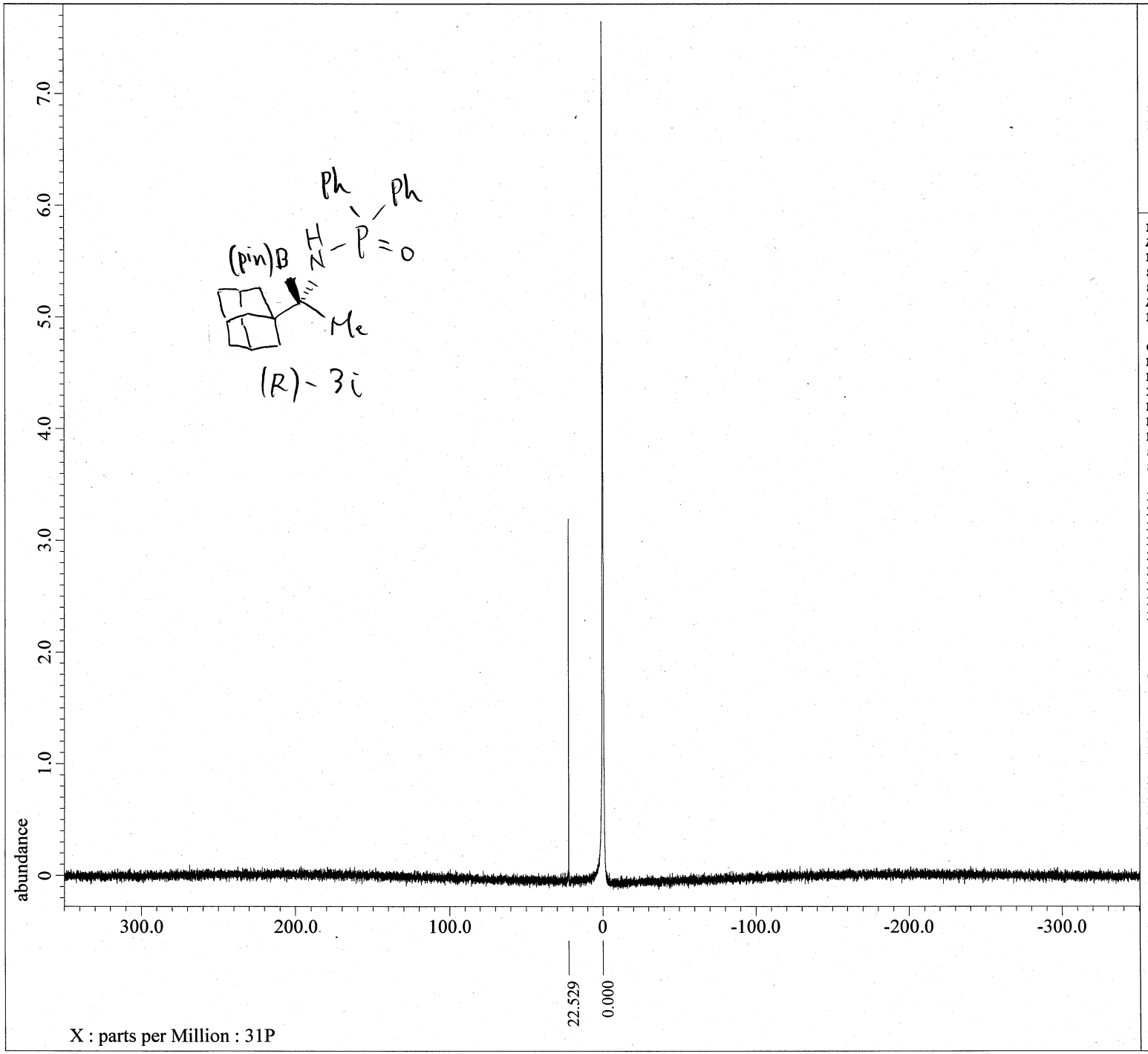

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-260-proton---1.jdf
Filename = MUR-260-proton---3.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-NOV-2020 05:27:13
Revision_Time = 31-JAN-2021 19:19:36
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 2.20725248[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45305193[Hz]
X_Sweep = 7.42280285[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 20.8[dC]
X_90_Width = 12.6[us]
X_Acq_Time = 2.20725248[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 6.3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.20725248[s]
abundance
X : parts per Million : 1H
7.862 7.859 7.848 7.831 7.828 7.816 7.800 7.444 7.426 7.419 7.416 7.411 7.408 7.401 7.265
3.064 3.044
2.018
1.663 1.631 1.331 1.295 1.136
0.000
Me
(R)-3i


---- 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: MUR-260-13C-2.jdf
Filename = MUR-260-13C-3.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-NOV-2020 05:29:52
Revision_Time = 31-JAN-2021 19:18:33
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 4000
Total_Scans = 4000
Relaxation_Delay = 2[s]
Recvr_Gain = 52
Temp_Get = 21.5[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[s]
(R)-3i
Me
abundance
X : parts per Million : 13C
137.008
132.017
131.921
131.758
131.662
131.241
131.222
131.174
131.145
128.415
128.396
128.290
128.271
84.269
77.486
77.160
76.844
52.998
37.440
37.354
28.808
25.168
15.539
15.491



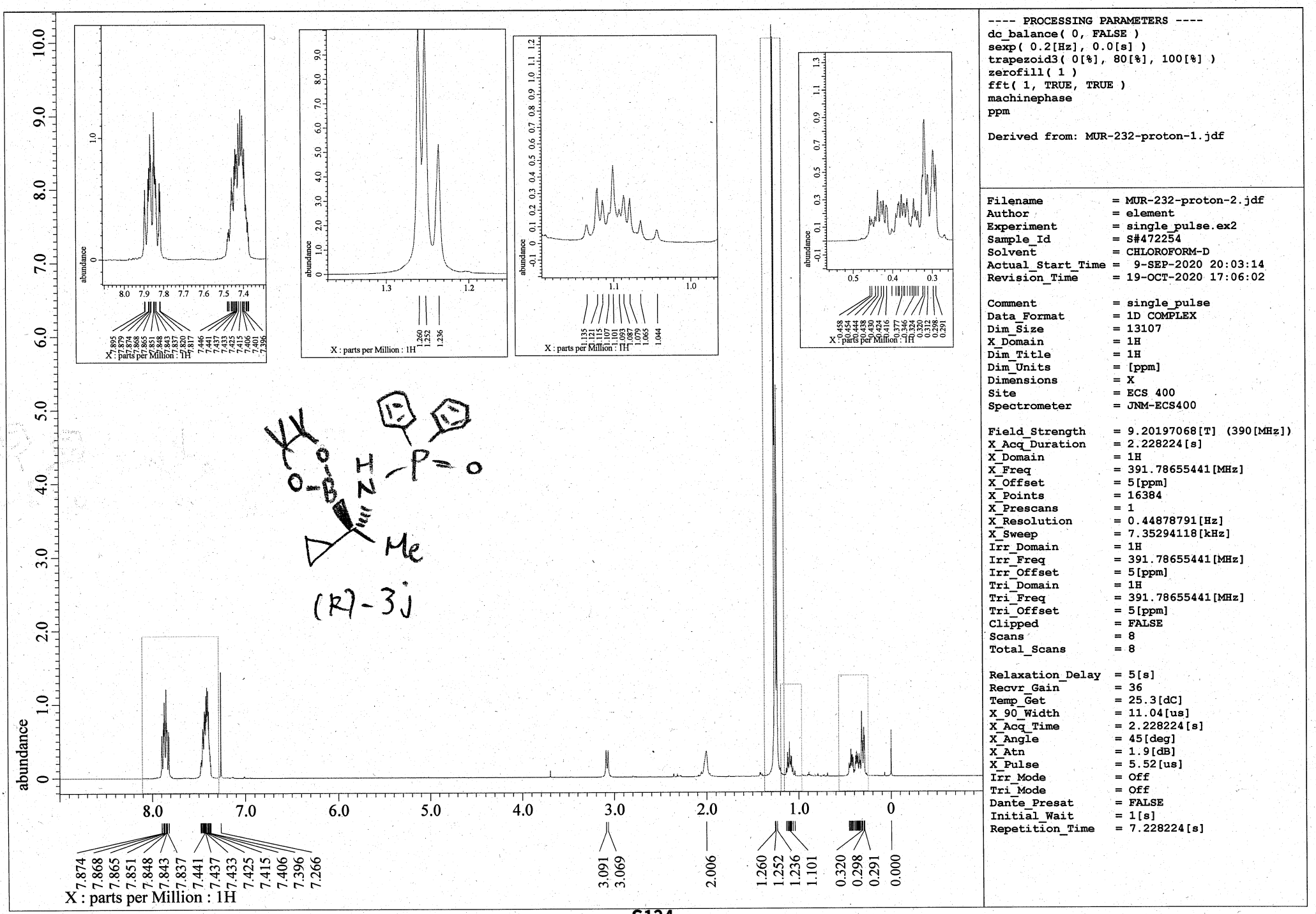

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-260-11B-1.jdf
```

```
Filename            = MUR-260-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#571637
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  4-MAR-2021 00:00:33
Revision_Time       =  4-MAR-2021 15:37:38

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 449
Total_Scans         = 449

Relaxation_Delay    = 2[s]
Recvr_Gain          = 56
Temp_Get            = 19[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```



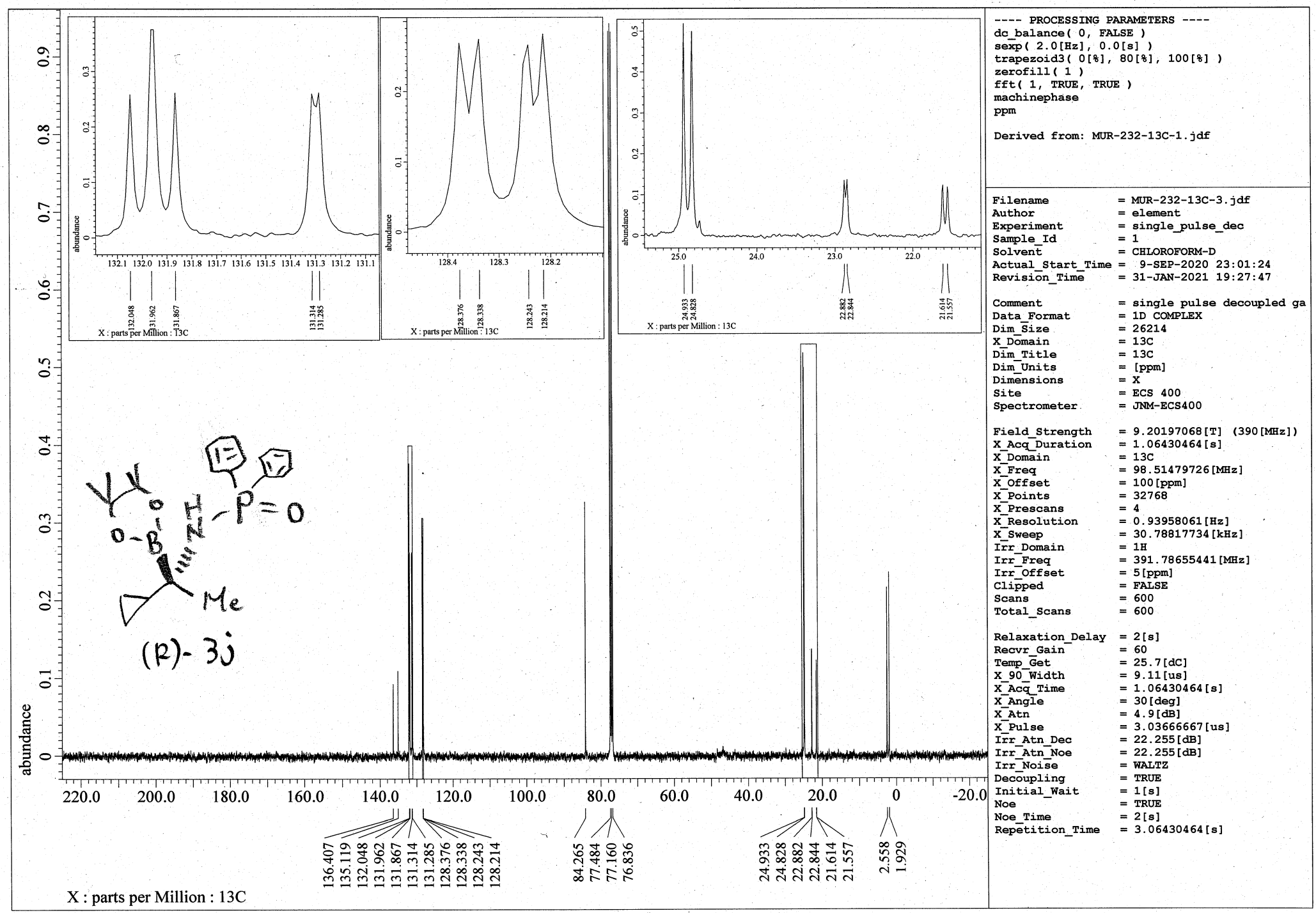

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-260-31P-1.jdf
```

```
Filename            = MUR-260-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#488095
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 20:19:18
Revision_Time       =  6-MAY-2021 21:29:45

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```



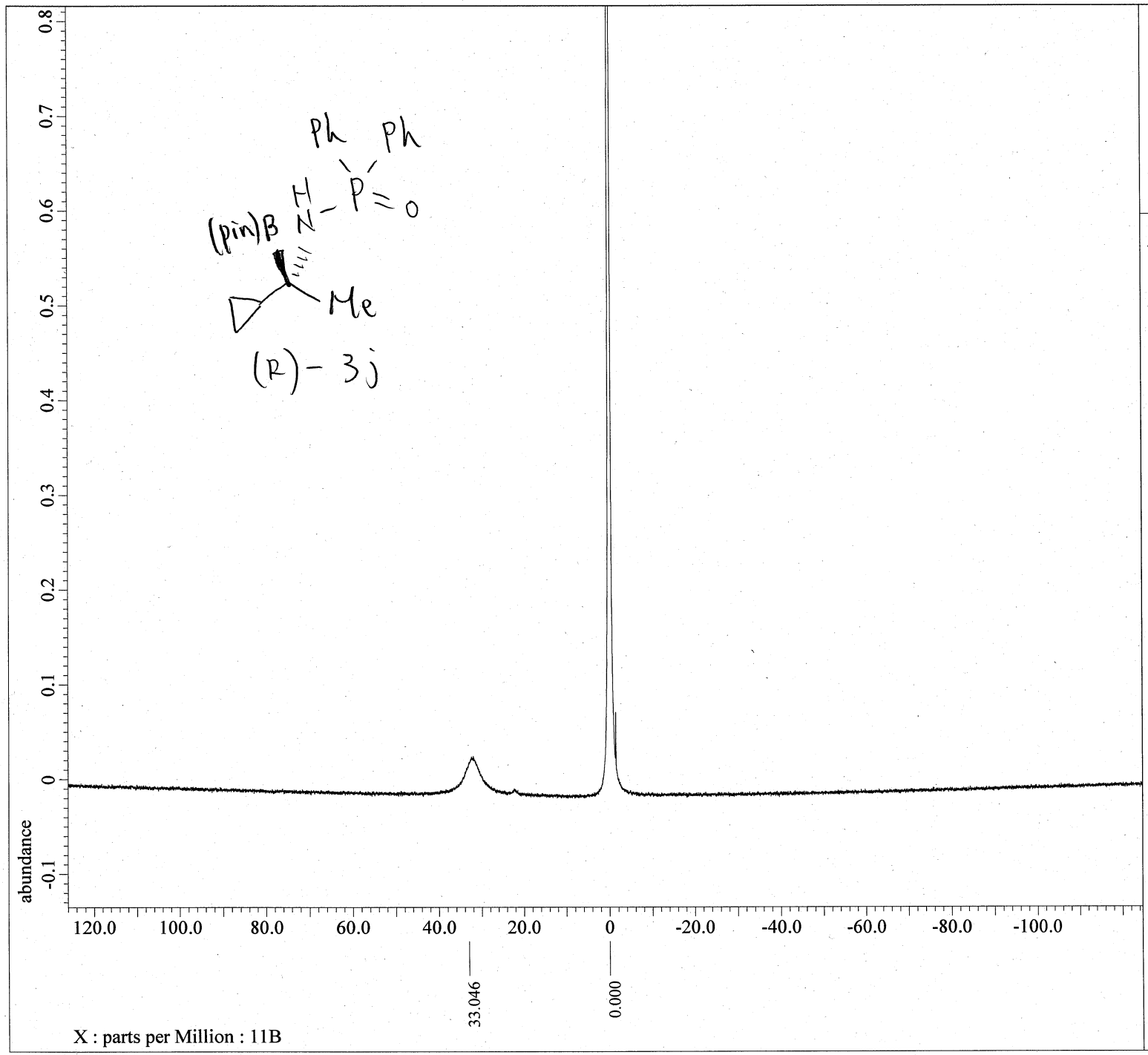

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-232-proton-1.jdf
```

Filename	= MUR-232-proton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#472254
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-SEP-2020 20:03:14
Revision_Time	= 19-OCT-2020 17:06:02
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	= 36
Temp_Get	= 25.3[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]



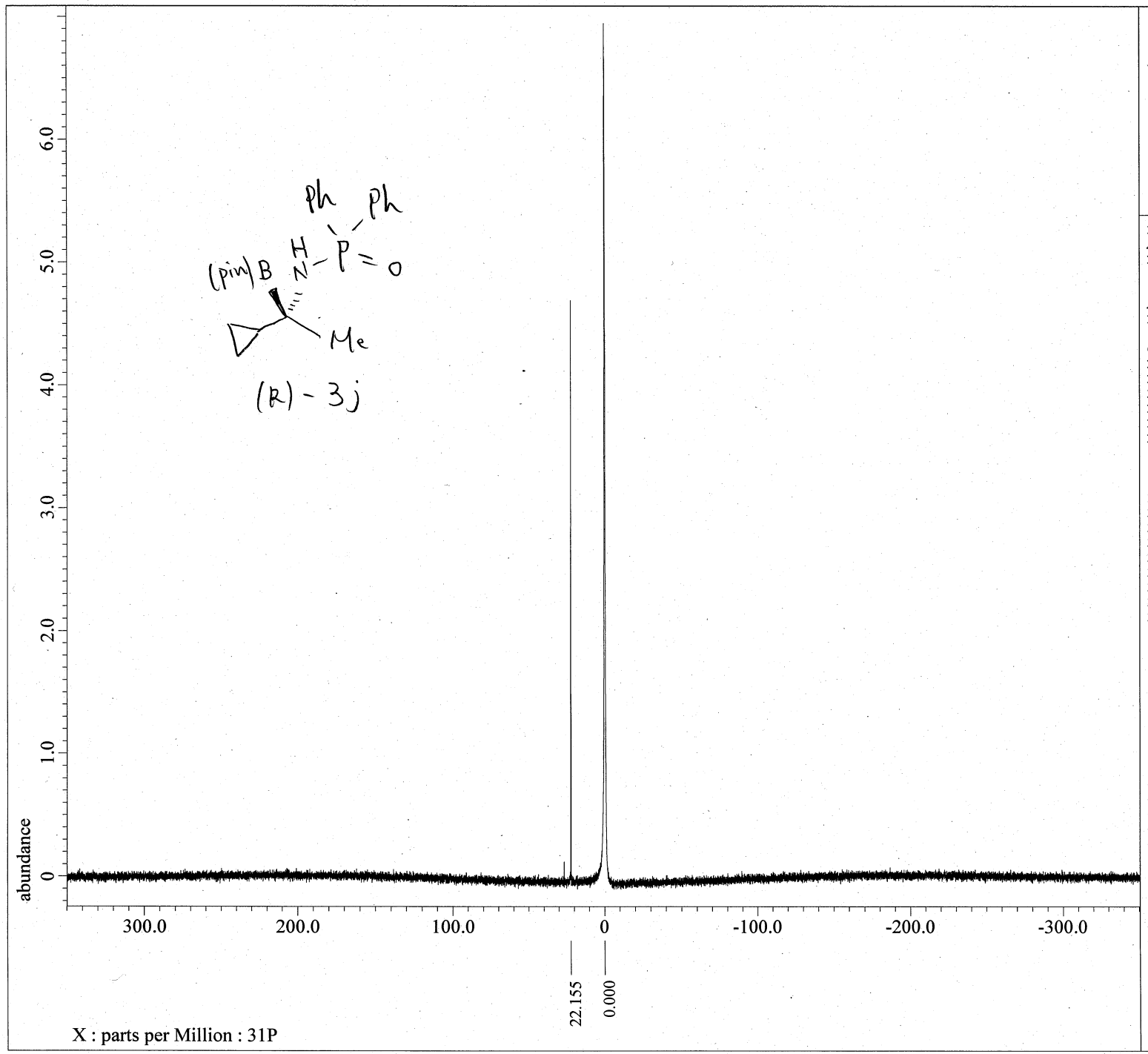

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-232-13C-1.jdf
```

Filename	= MUR-232-13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-SEP-2020 23:01:24
Revision_Time	= 31-JAN-2021 19:27:47
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 600
Total_Scans	= 600
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 25.7[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]



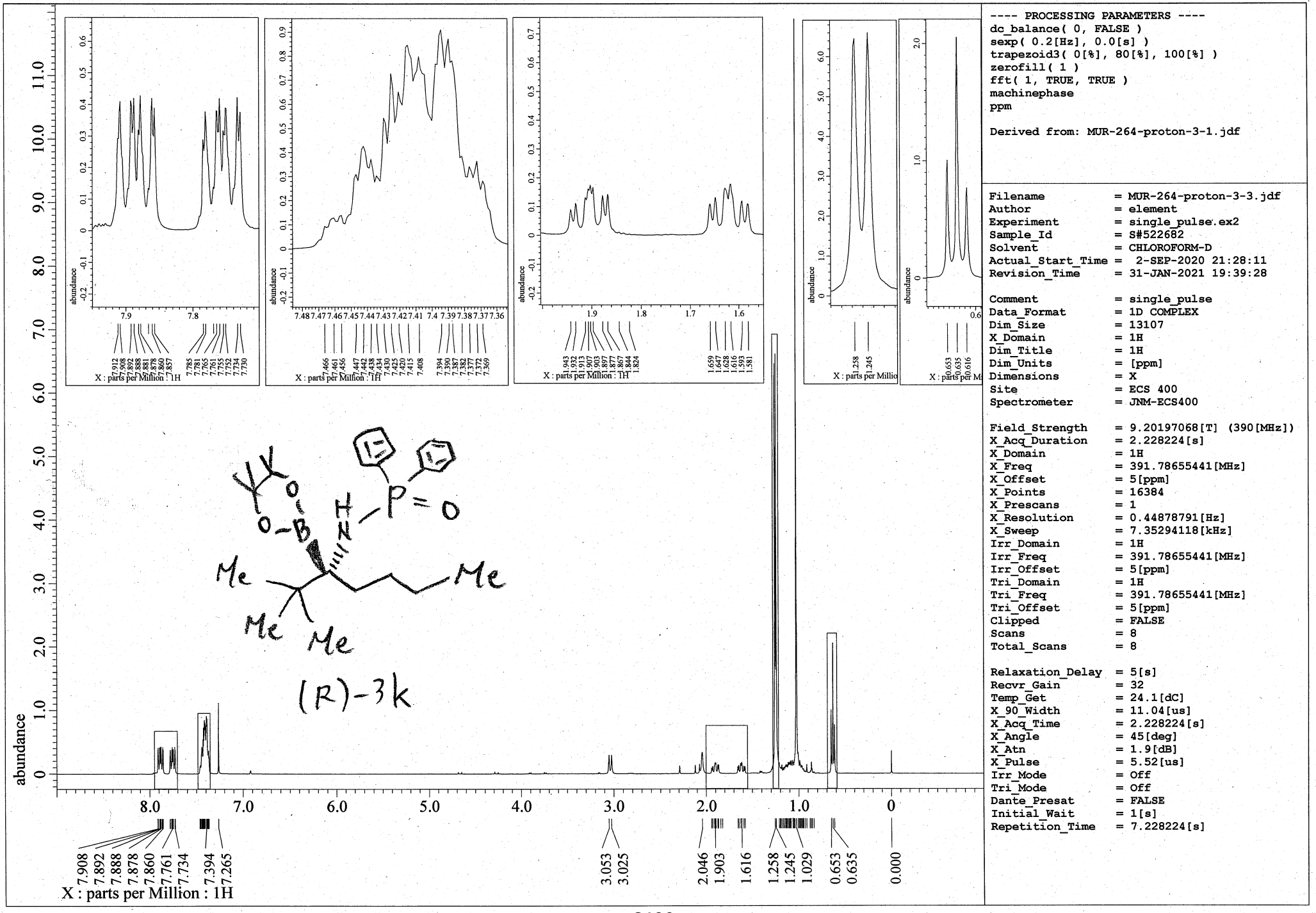

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-232-11B-1.jdf
```

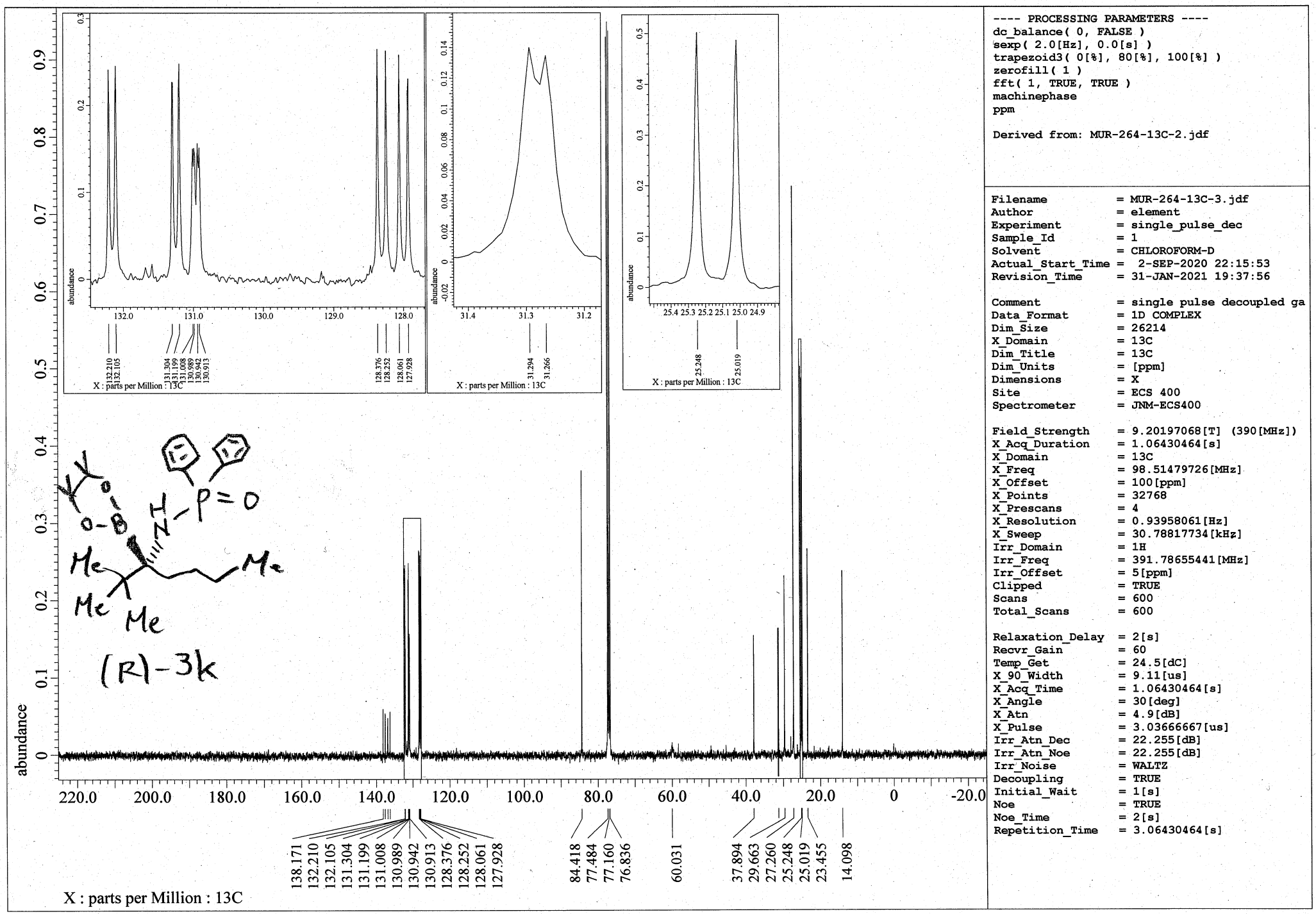
```
Filename            = MUR-232-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#743137
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  4-MAR-2021 04:45:57
Revision_Time       =  4-MAR-2021 15:34:41

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 770
Total_Scans         = 770

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20.6[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```

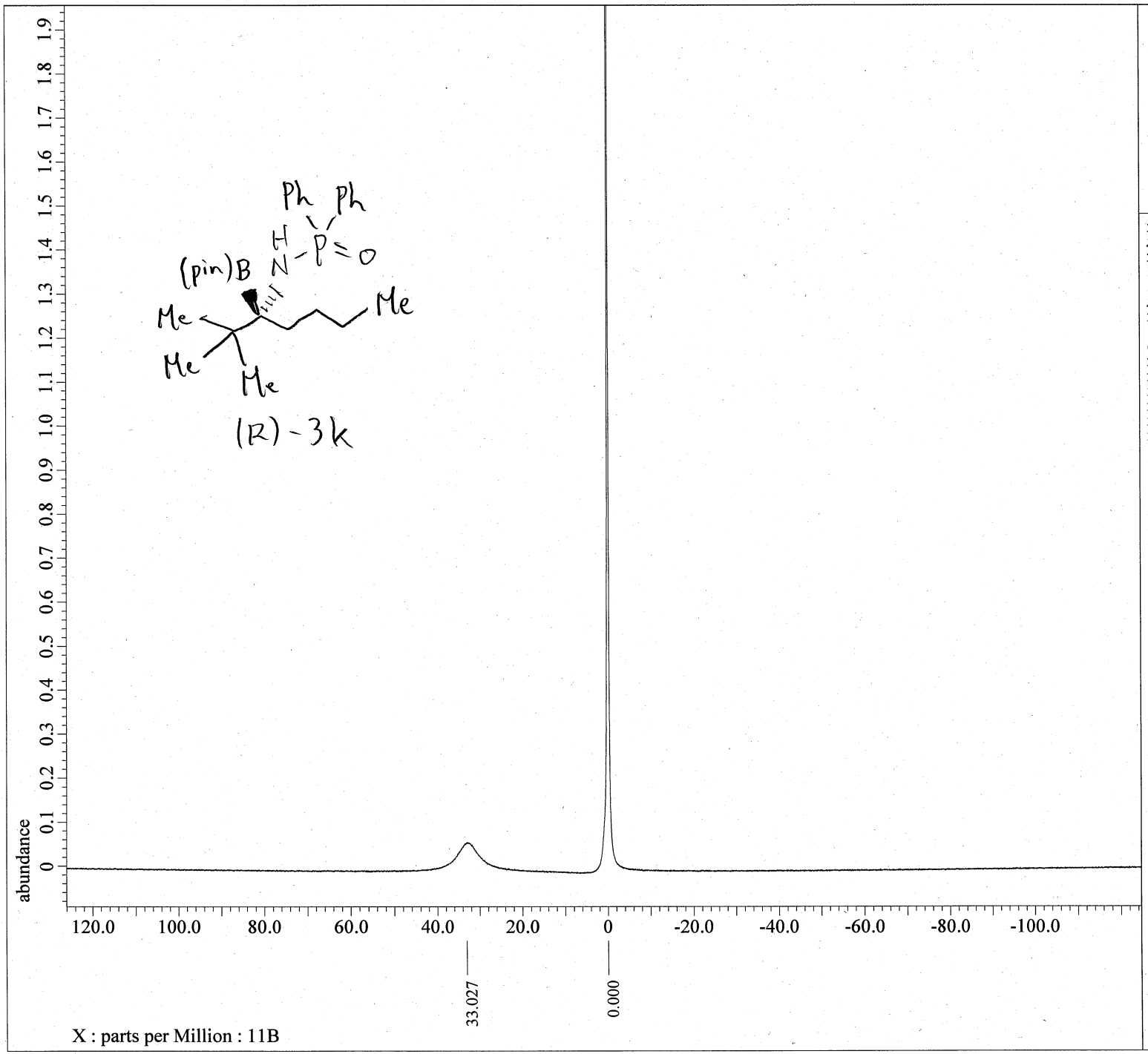



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-232-31P-1.jdf
```

```
Filename            = MUR-232-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#565374
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 22:28:58
Revision_Time       =  6-MAY-2021 21:36:36

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 48
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```

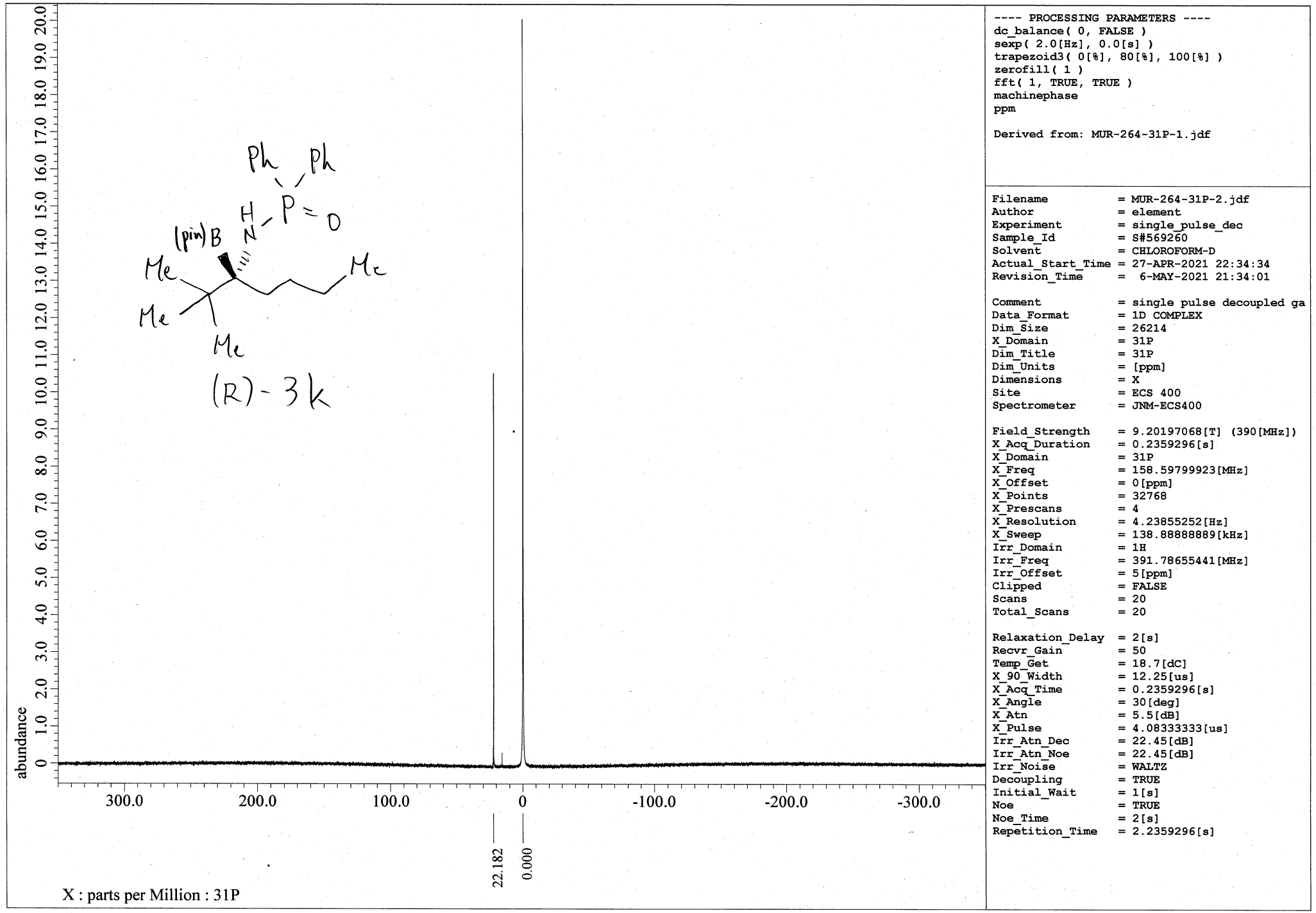

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-264-proton-3-1.jdf
Filename = MUR-264-proton-3-3.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#522682
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-SEP-2020 21:28:11
Revision_Time = 31-JAN-2021 19:39:28
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 = 32
Temp_Get = 24.1[dC]
X_90_Width = 11.04[us]
X_Acq_Time = 2.228224[s]
X_Angle = 45[deg]
X_Atn = 1.9[dB]
X_Pulse = 5.52[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.228224[s]
abundance
X : parts per Million : 1H
7.908 7.892 7.888 7.878 7.860 7.761 7.734 7.394 7.265
3.053 3.025
2.046 1.903 1.616 1.258 1.245 1.029
0.653 0.635
0.000
Me
Me
Me
Me
(R)-3k


abundance
X : parts per Million : 13C
(R)-3k
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-264-13C-2.jdf
Filename = MUR-264-13C-3.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-SEP-2020 22:15:53
Revision_Time = 31-JAN-2021 19:37:56
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 600
Total_Scans = 600
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.5[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]



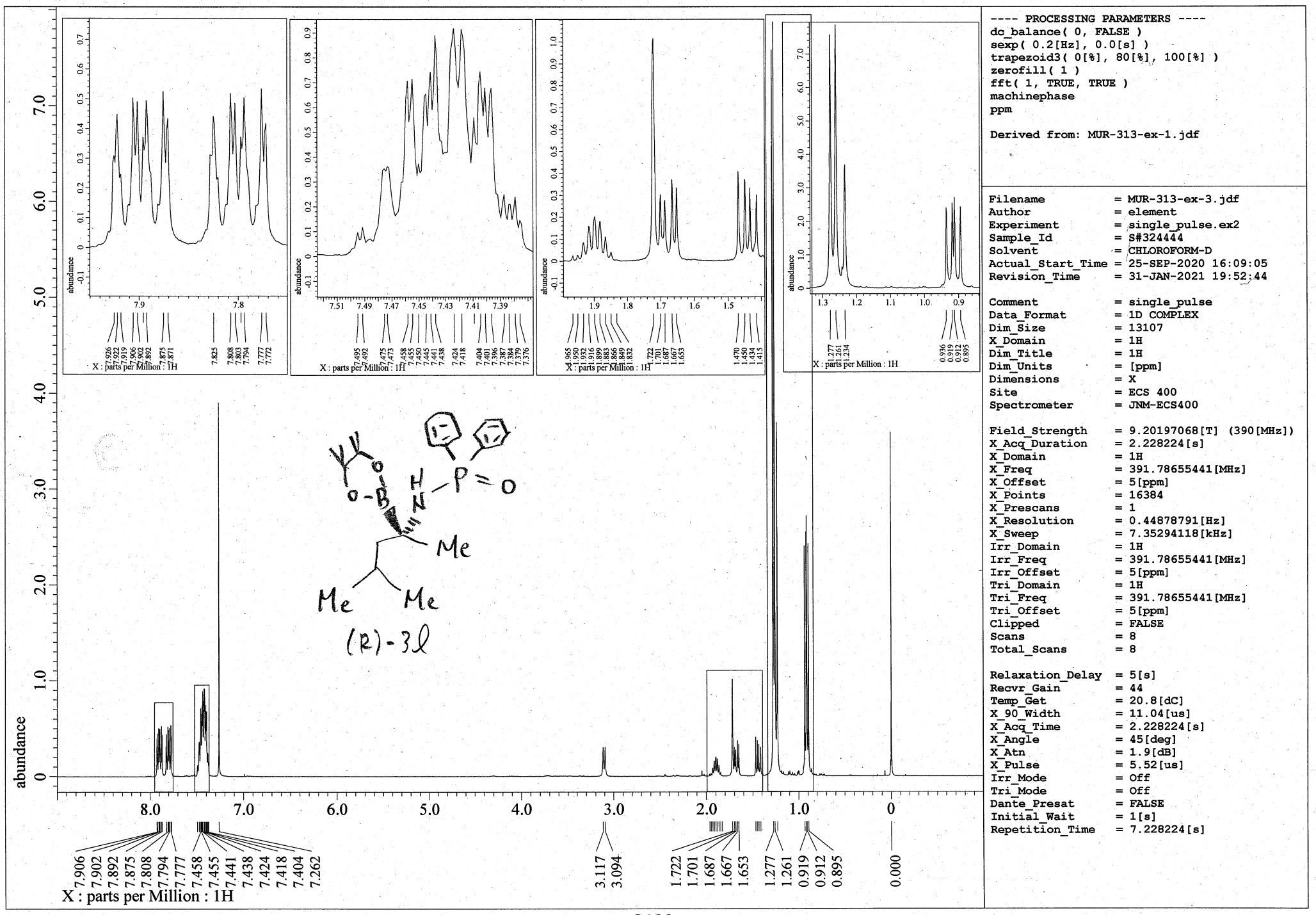

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-264-11B-1.jdf
```

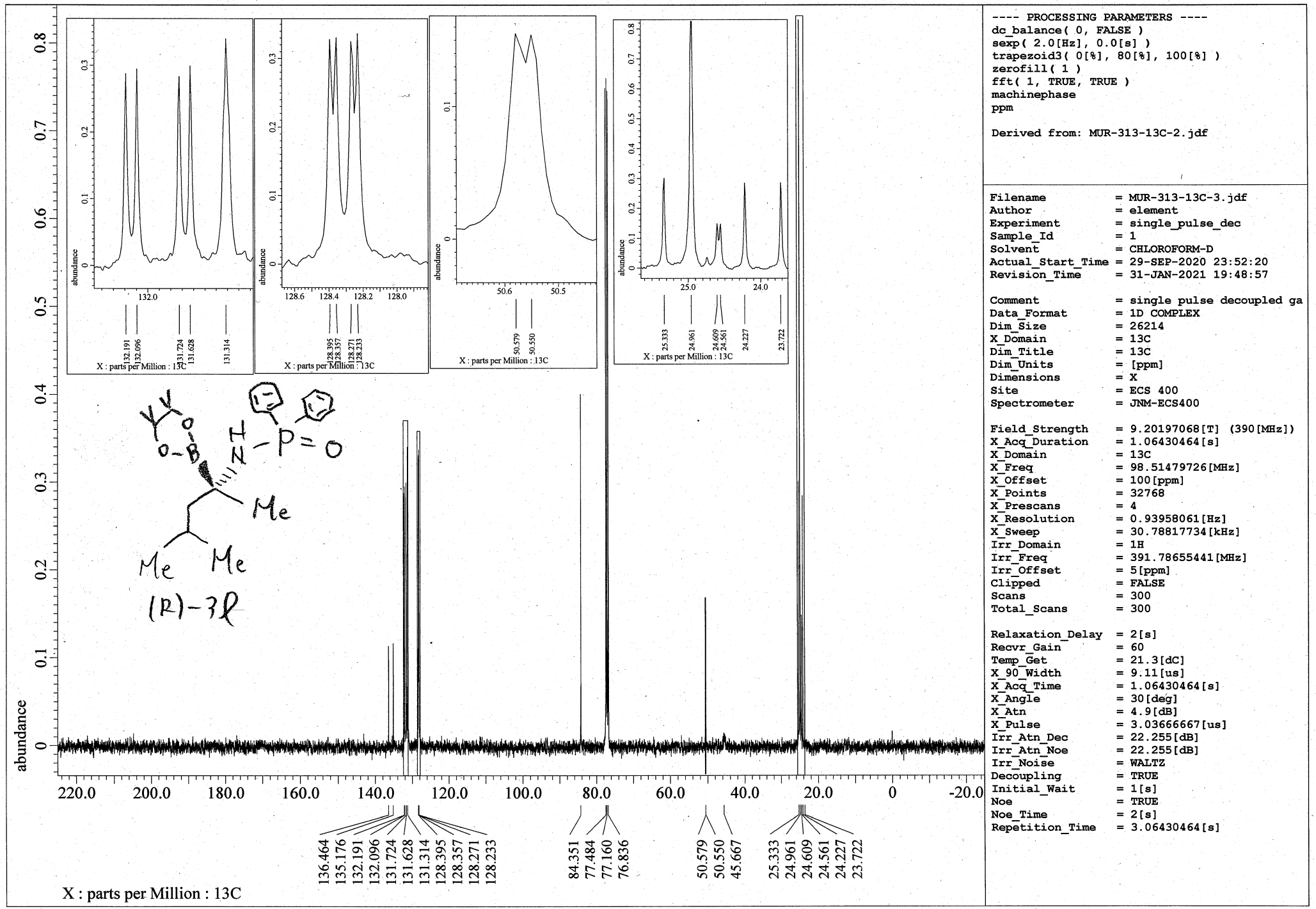
Filename	= MUR-264-11B-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#768828
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-MAR-2021 05:28:47
Revision_Time	= 4-MAR-2021 15:22:12
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 11B
Dim_Title	= 11B
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 0.82313216[s]
X_Domain	= 11B
X_Freq	= 127.01553457[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.21487174[Hz]
X_Sweep	= 39.8089172[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1000
Total_Scans	= 1000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.4[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 0.82313216[s]
X_Angle	= 30[deg]
X_Atn	= 4.8[dB]
X_Pulse	= 3.33333333[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Atn_Noe	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.82313216[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

Derived from: MUR-264-31P-1.jdf
```

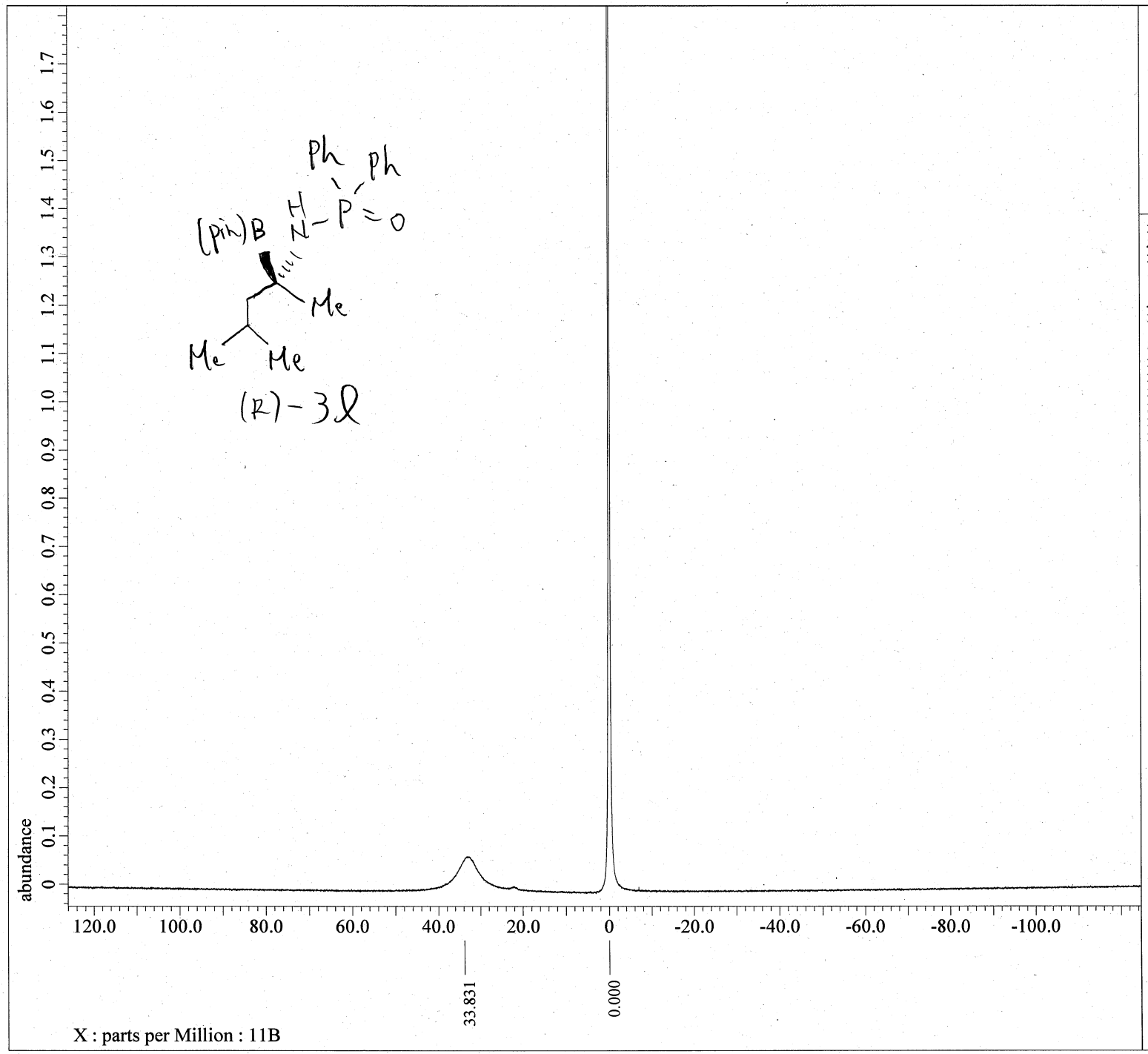
```
Filename            = MUR-264-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#569260
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 22:34:34
Revision_Time       =  6-MAY-2021 21:34:01

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[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
Derived from: MUR-313-ex-1.jdf
Filename = MUR-313-ex-3.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#324444
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-SEP-2020 16:09:05
Revision_Time = 31-JAN-2021 19:52:44
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 = 44
Temp_Get = 20.8[dC]
X_90_Width = 11.04[us]
X_Acq_Time = 2.228224[s]
X_Angle = 45[deg]
X_Atn = 1.9[dB]
X_Pulse = 5.52[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.228224[s]
Me
Me
Me
(R)-3l
abundance
X : parts per Million : 1H
7.906
7.902
7.892
7.875
7.808
7.794
7.777
7.458
7.455
7.441
7.438
7.424
7.418
7.404
7.262
3.117
3.094
1.722
1.701
1.687
1.667
1.653
1.277
1.261
0.919
0.912
0.895
0.000



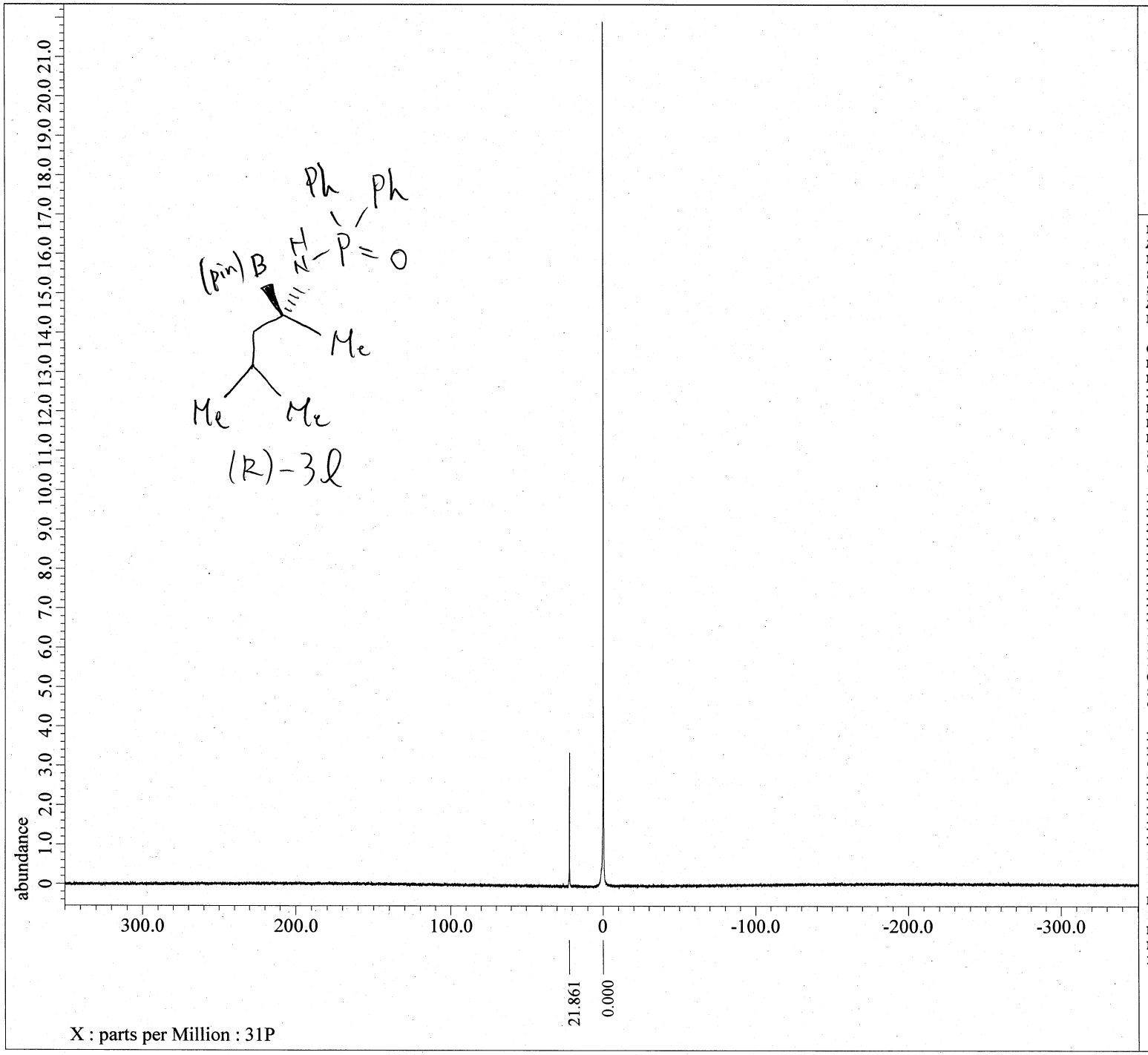

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-313-13C-2.jdf
```

Filename	= MUR-313-13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-SEP-2020 23:52:20
Revision_Time	= 31-JAN-2021 19:48:57
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 300
Total_Scans	= 300
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]



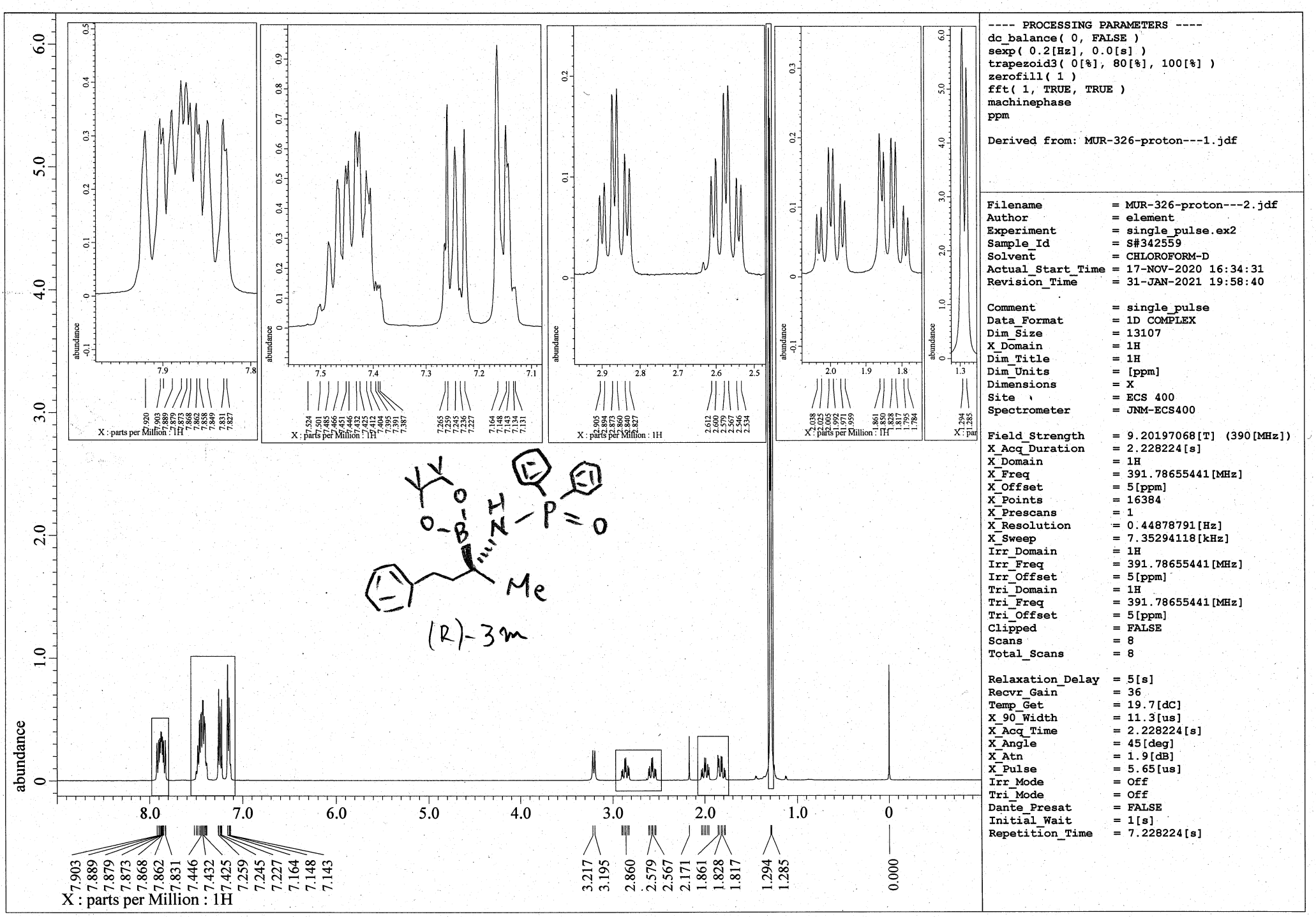

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-313-11B-1.jdf
```

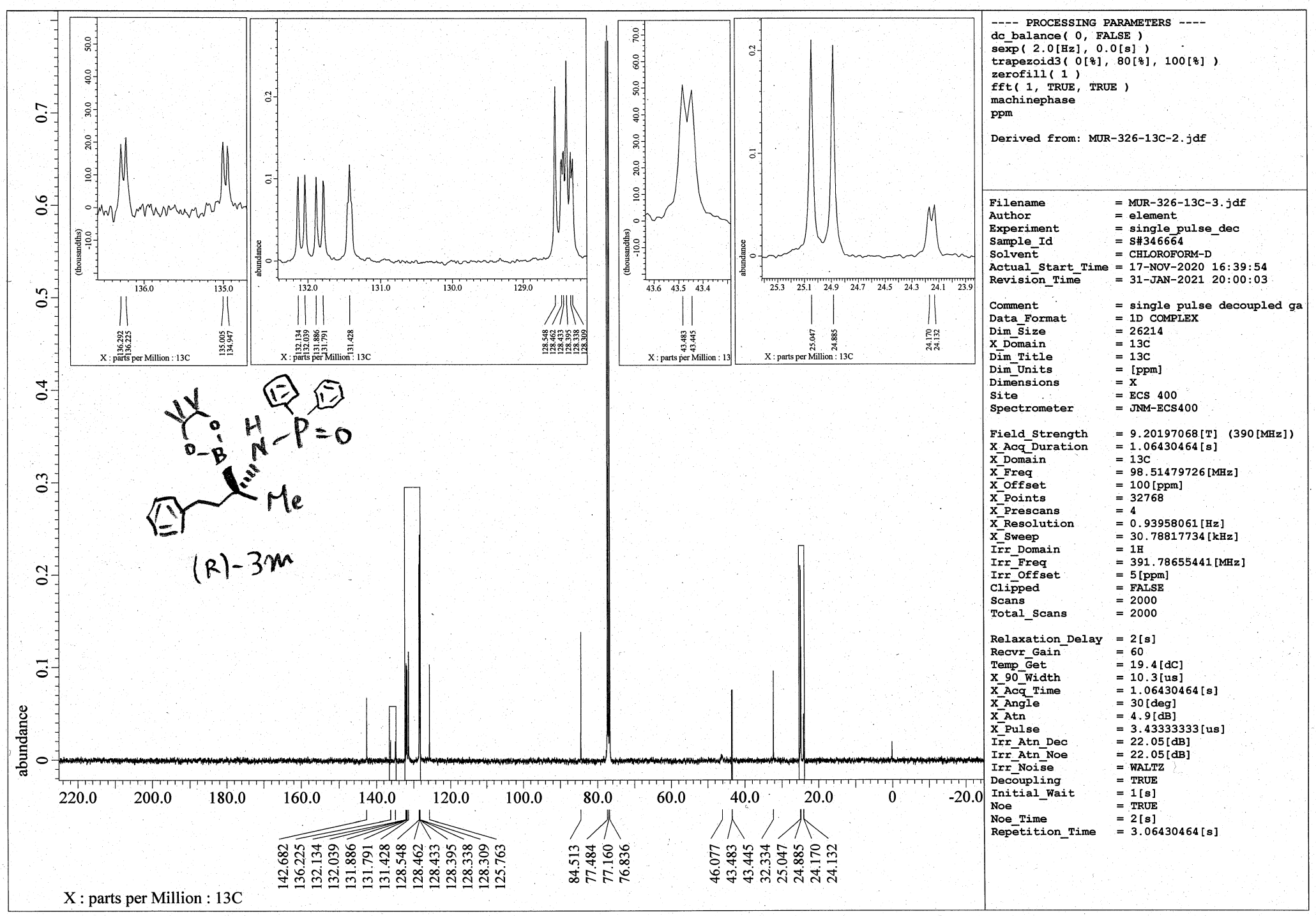
Filename	= MUR-313-11B-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#481754
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-MAR-2021 21:30:26
Revision_Time	= 4-MAR-2021 15:39:26
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 11B
Dim_Title	= 11B
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 0.82313216[s]
X_Domain	= 11B
X_Freq	= 127.01553457[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.21487174[Hz]
X_Sweep	= 39.8089172[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 500
Total_Scans	= 500
Relaxation_Delay	= 2[s]
Recvr_Gain	= 48
Temp_Get	= 20.2[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 0.82313216[s]
X_Angle	= 30[deg]
X_Atn	= 4.8[dB]
X_Pulse	= 3.33333333[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Atn_Noe	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.82313216[s]

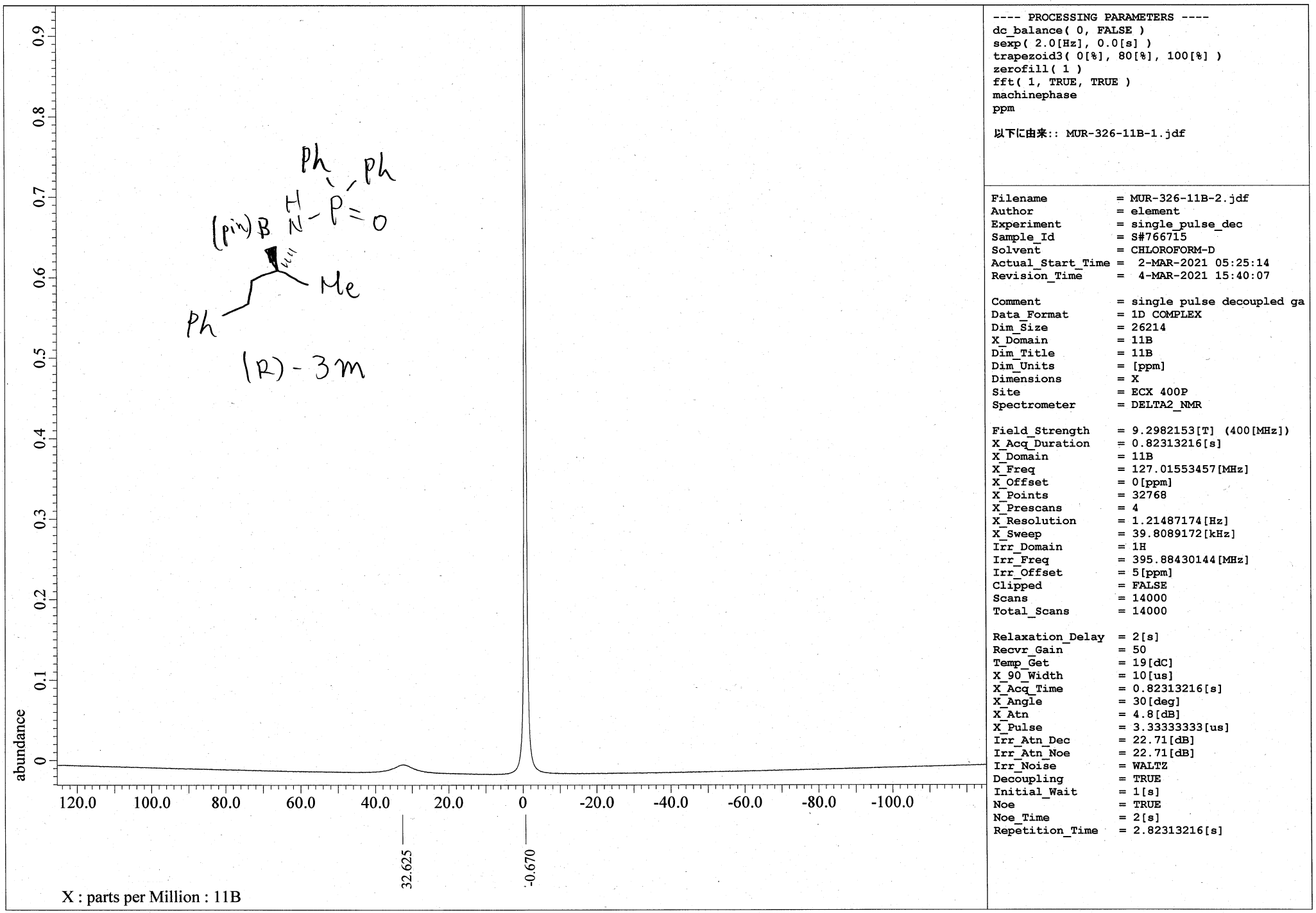



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-313-31P-1.jdf
```

```
Filename            = MUR-313-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#572735
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-APR-2021 22:40:26
Revision_Time       =  6-MAY-2021 21:35:09

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 48
Temp_Get            = 18.7[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```

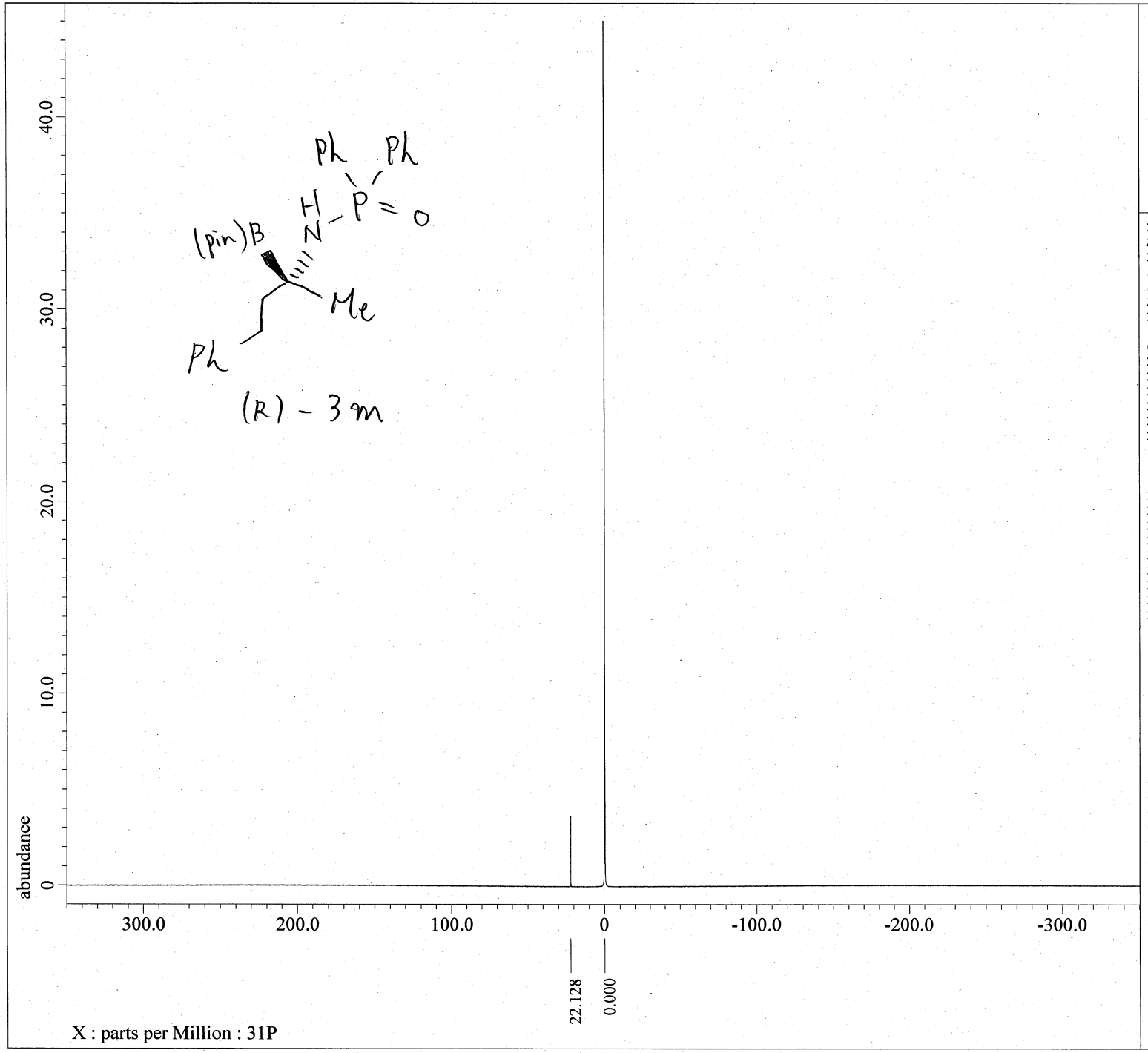

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MUR-326-proton---1.jdf
Filename = MUR-326-proton---2.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#342559
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-NOV-2020 16:34:31
Revision_Time = 31-JAN-2021 19:58:40
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 2.228224[s]
X_Domain = 1H
X_Freq = 391.78655441[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.44878791[Hz]
X_Sweep = 7.35294118[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 391.78655441[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 19.7[dC]
X_90_Width = 11.3[us]
X_Acq_Time = 2.228224[s]
X_Angle = 45[deg]
X_Atn = 1.9[dB]
X_Pulse = 5.65[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.228224[s]
Me
(R)-3m
abundance
X : parts per Million : 1H
7.903 7.889 7.879 7.873 7.868 7.862 7.831 7.446 7.432 7.425 7.259 7.245 7.227 7.164 7.148 7.143
3.217 3.195 2.860 2.579 2.567 2.171 1.861 1.828 1.817 1.294 1.285 0.000


---- 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: MUR-326-13C-2.jdf
Filename = MUR-326-13C-3.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#346664
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-NOV-2020 16:39:54
Revision_Time = 31-JAN-2021 20:00:03
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 2000
Total_Scans = 2000
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.4[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.43333333[us]
Irr_Atn_Dec = 22.05[dB]
Irr_Atn_Noe = 22.05[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
(R)-3m
Me
abundance
X : parts per Million : 13C
142.682
136.225
132.134
132.039
131.886
131.791
131.428
128.548
128.462
128.433
128.395
128.338
128.309
125.763
84.513
77.484
77.160
76.836
46.077
43.483
43.445
32.334
25.047
24.885
24.170
24.132



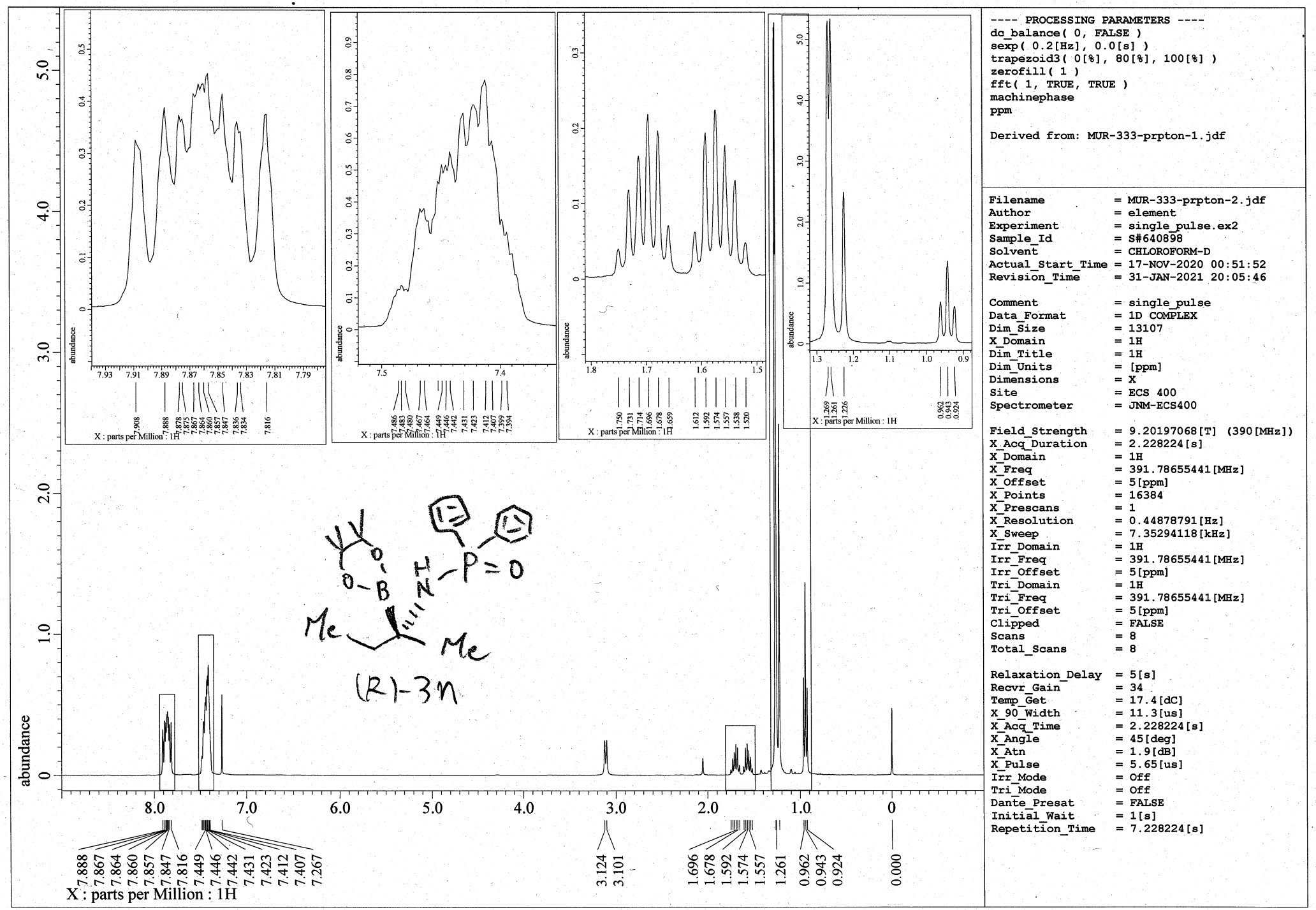

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-326-11B-1.jdf
```

Filename	= MUR-326-11B-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#766715
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-MAR-2021 05:25:14
Revision_Time	= 4-MAR-2021 15:40:07
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 11B
Dim_Title	= 11B
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 0.82313216[s]
X_Domain	= 11B
X_Freq	= 127.01553457[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.21487174[Hz]
X_Sweep	= 39.8089172[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 14000
Total_Scans	= 14000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 0.82313216[s]
X_Angle	= 30[deg]
X_Atn	= 4.8[dB]
X_Pulse	= 3.33333333[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Atn_Noe	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.82313216[s]



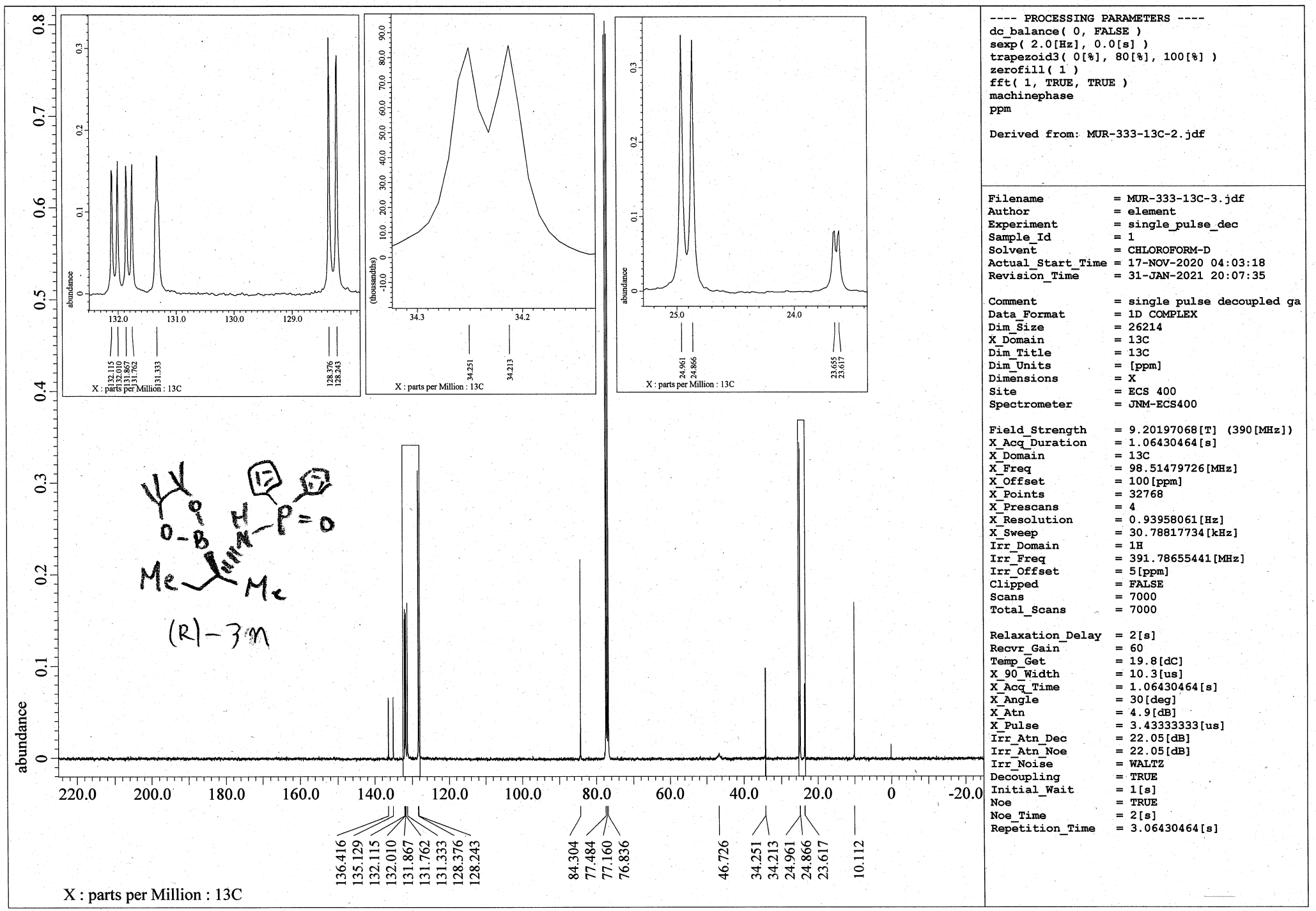

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-326-31P-1.jdf
```

```
Filename            = MUR-326-31P-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#533729
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-APR-2021 21:36:18
Revision_Time       =  6-MAY-2021 21:30:38

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 31P
Dim_Title           = 31P
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.2359296[s]
X_Domain            = 31P
X_Freq              = 158.59799923[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.23855252[Hz]
X_Sweep             = 138.88888889[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          = 50
Temp_Get            = 18.9[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 0.2359296[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 4.08333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.2359296[s]
```



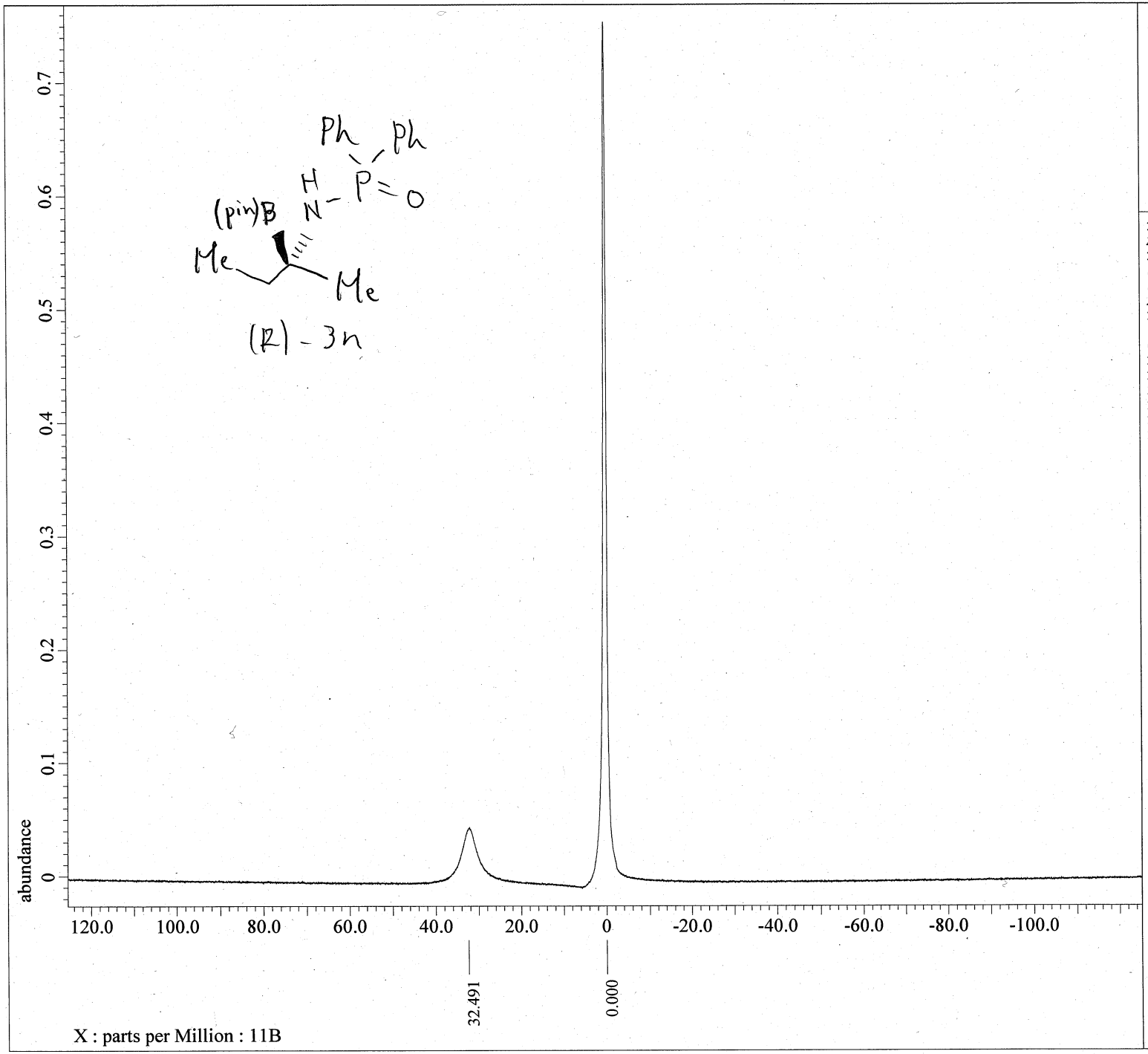

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-333-prpton-1.jdf
```

Filename	= MUR-333-prpton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#640898
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-NOV-2020 00:51:52
Revision_Time	= 31-JAN-2021 20:05:46
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 34
Temp_Get	= 17.4[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]



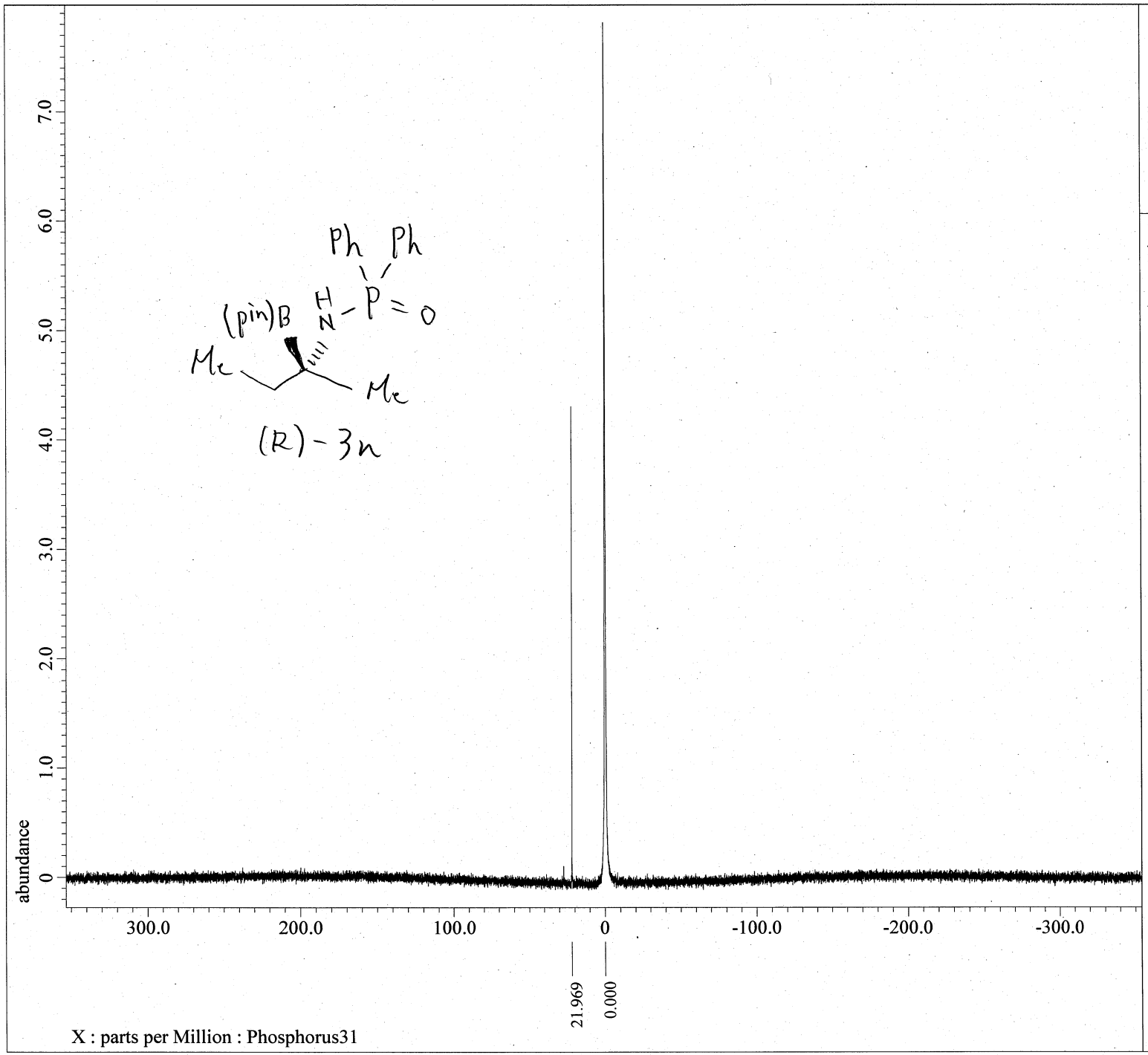

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-333-13C-2.jdf
```

Filename	= MUR-333-13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-NOV-2020 04:03:18
Revision_Time	= 31-JAN-2021 20:07:35
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 7000
Total_Scans	= 7000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.8[dC]
X_90_Width	= 10.3[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.43333333[us]
Irr_Atn_Dec	= 22.05[dB]
Irr_Atn_Noe	= 22.05[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



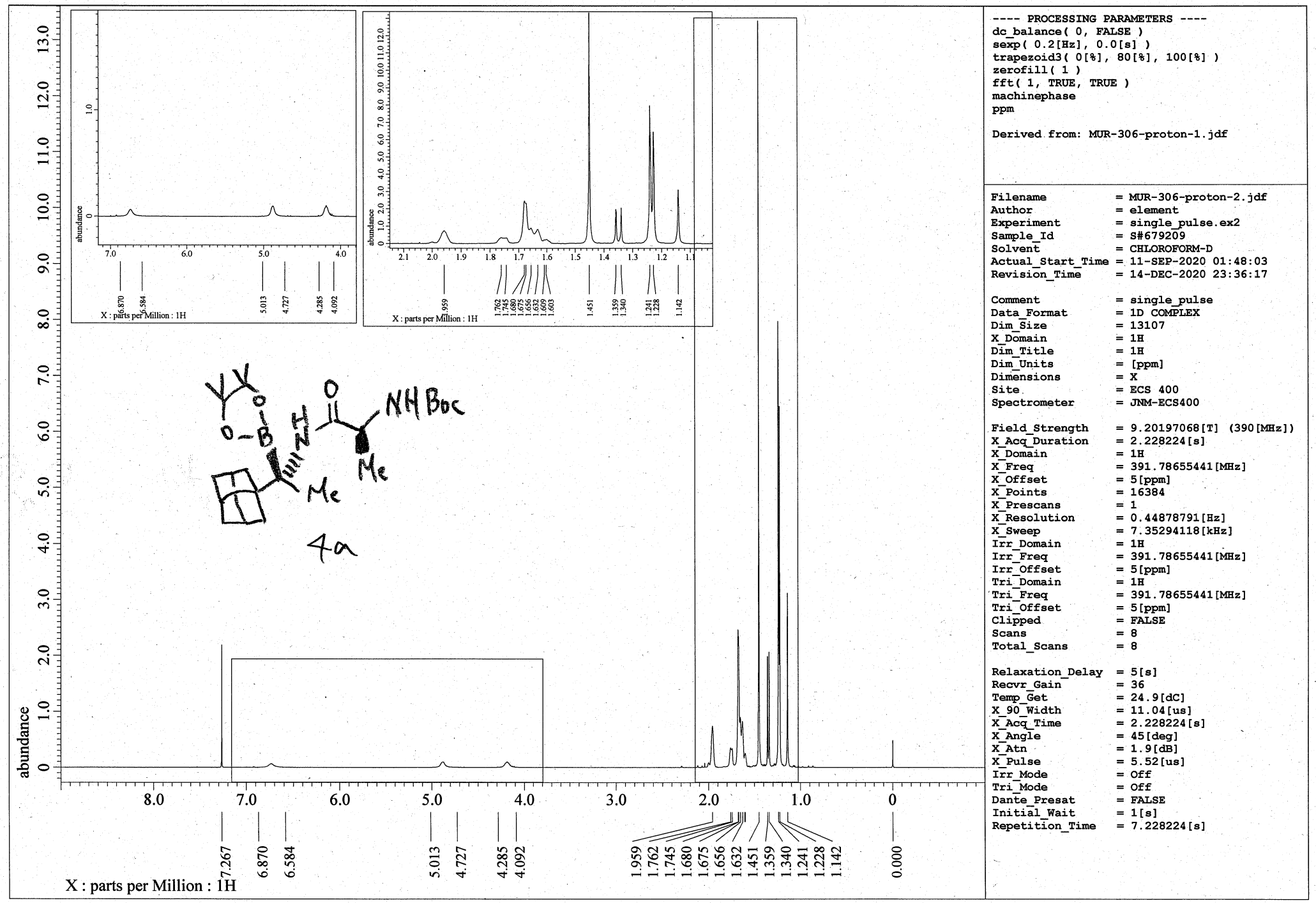

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-333-11B-1.jdf
```

```
Filename            = MUR-333-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#768573
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-MAR-2021 05:29:07
Revision_Time       =  5-MAR-2021 09:18:56

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 14500
Total_Scans         = 14500

Relaxation_Delay    = 2[s]
Recvr_Gain          = 56
Temp_Get            = 19.9[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```



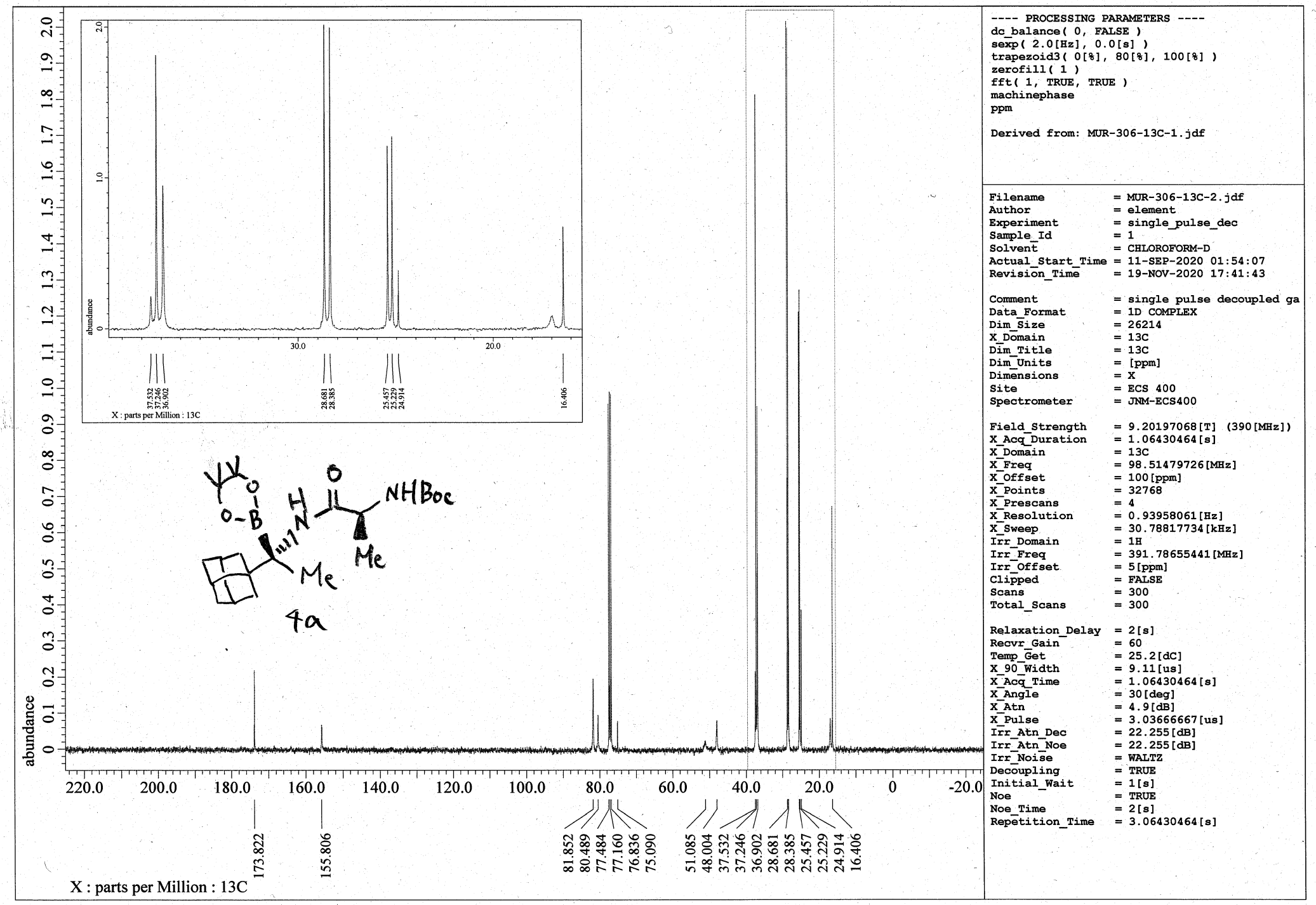

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MUR-333-31P_Carbon-1-1.jdf
```

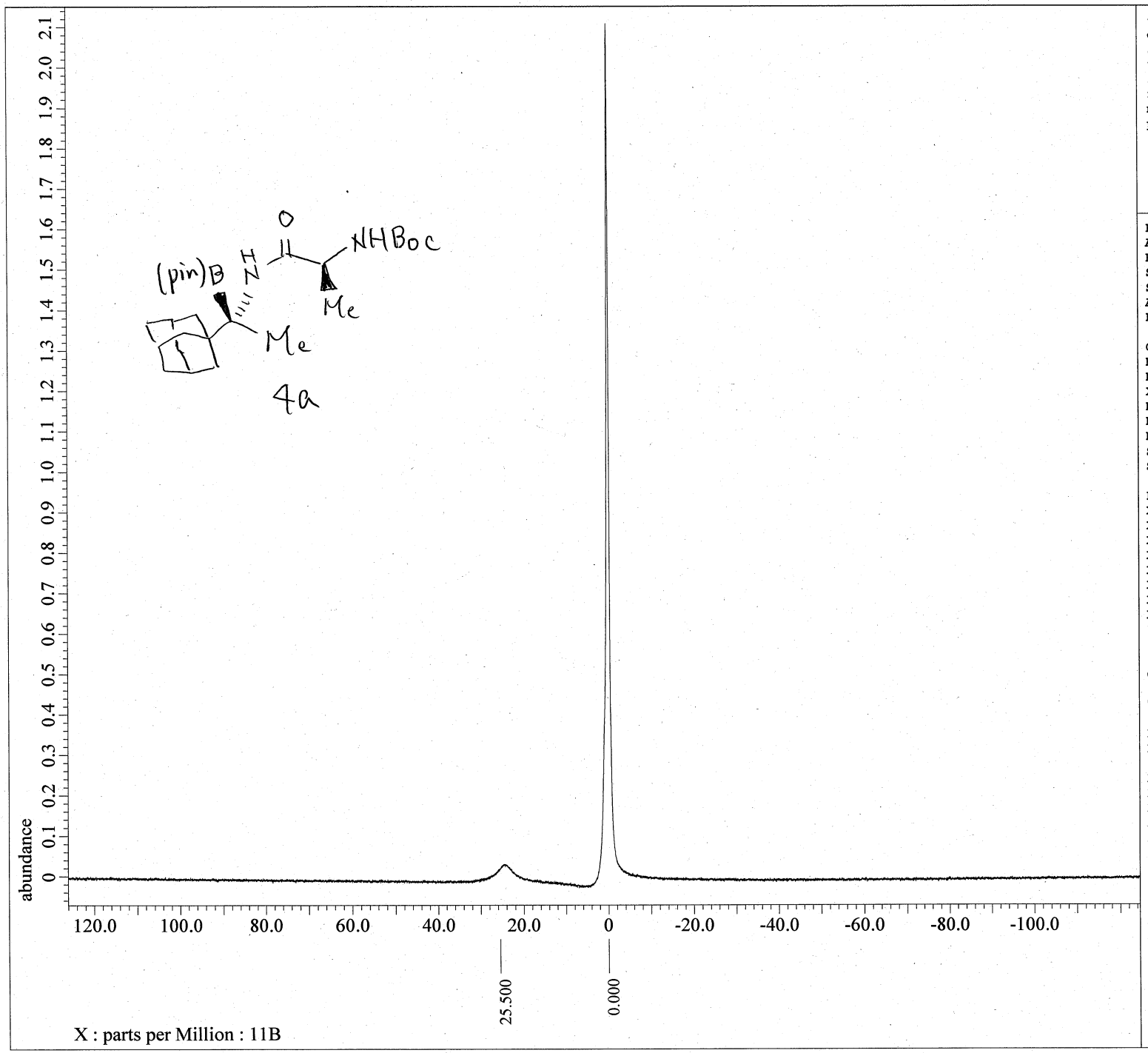
```
Filename            = MUR-333-31P_Carbon-1-2.jd
Author              = element
Experiment          = carbon.jxp
Sample_Id           = MUR-333-31P
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-APR-2021 16:34:41
Revision_Time       =  6-MAY-2021 21:31:05

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Phosph
Dim_Title           = Phosphorus31
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 0.229376[s]
X_Domain            = 31P
X_Freq              = 161.53211155[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 4.35965402[Hz]
X_Sweep             = 142.85714286[kHz]
X_Sweep_Clipped     = 114.28571429[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 20
Total_Scans         = 20

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.3[dC]
X_90_Width          = 16.75[us]
X_Acq_Time          = 0.229376[s]
X_Angle             = 30[deg]
X_Atn               = 4.7[dB]
X_Pulse             = 5.58333333[us]
Irr_Atn_Dec         = 25.823[dB]
Irr_Atn_Noe         = 25.823[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 0.115[ms]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.229376[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

Derived from: MUR-306-proton-1.jdf
```

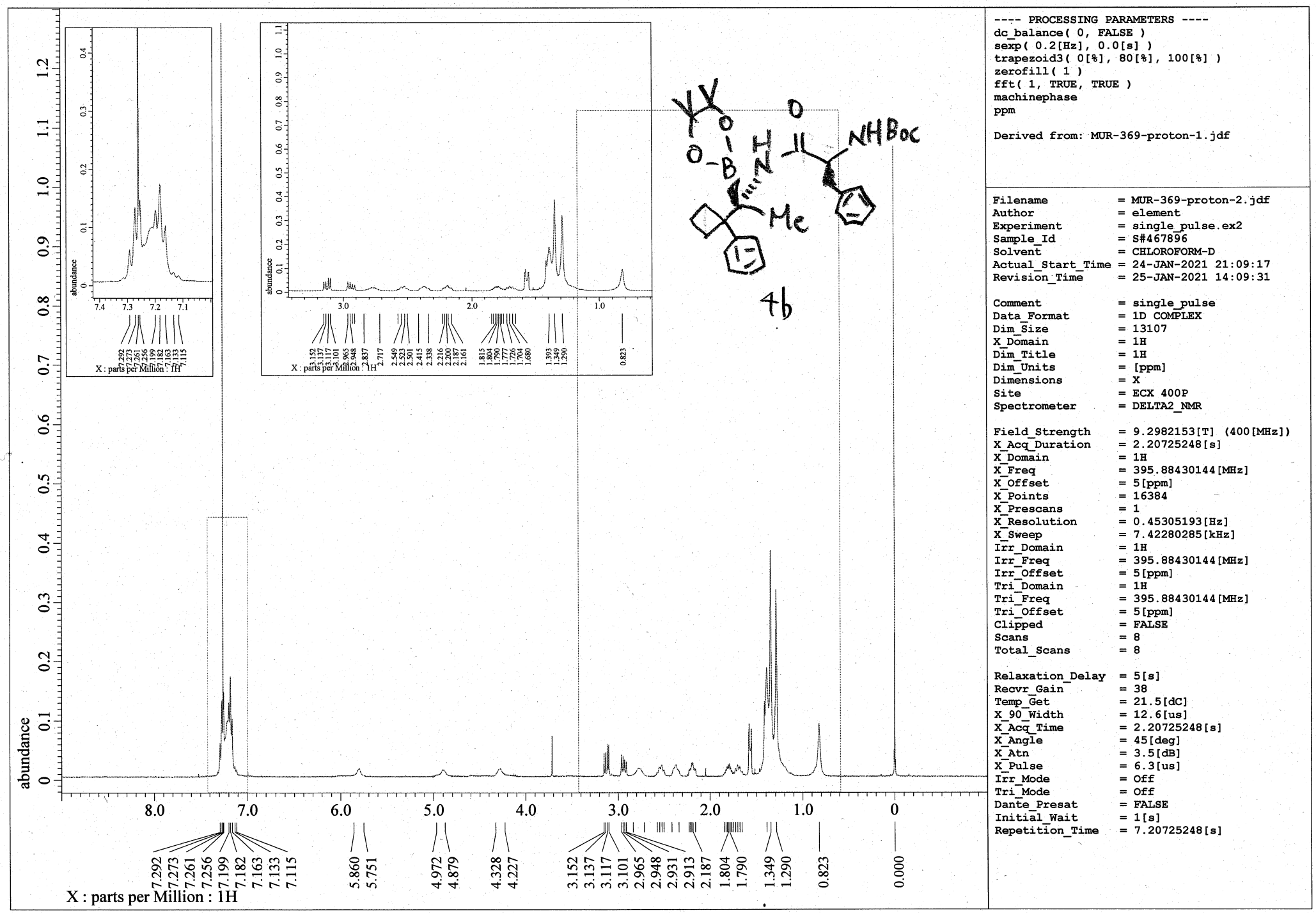
Filename	= MUR-306-proton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#679209
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-SEP-2020 01:48:03
Revision_Time	= 14-DEC-2020 23:36:17
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [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	= 36
Temp_Get	= 24.9[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]


---- 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: MUR-306-13C-1.jdf
Filename = MUR-306-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2020 01:54:07
Revision_Time = 19-NOV-2020 17:41:43
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 300
Total_Scans = 300
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25.2[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]
abundance
X : parts per Million : 13C
37.532
37.246
36.902
28.681
28.385
25.457
25.229
24.914
16.406
NHBoc
Me
Me
4a
173.822
155.806
81.852
80.489
77.484
77.160
76.836
75.090
51.085
48.004
37.532
37.246
36.902
28.681
28.385
25.457
25.229
24.914
16.406



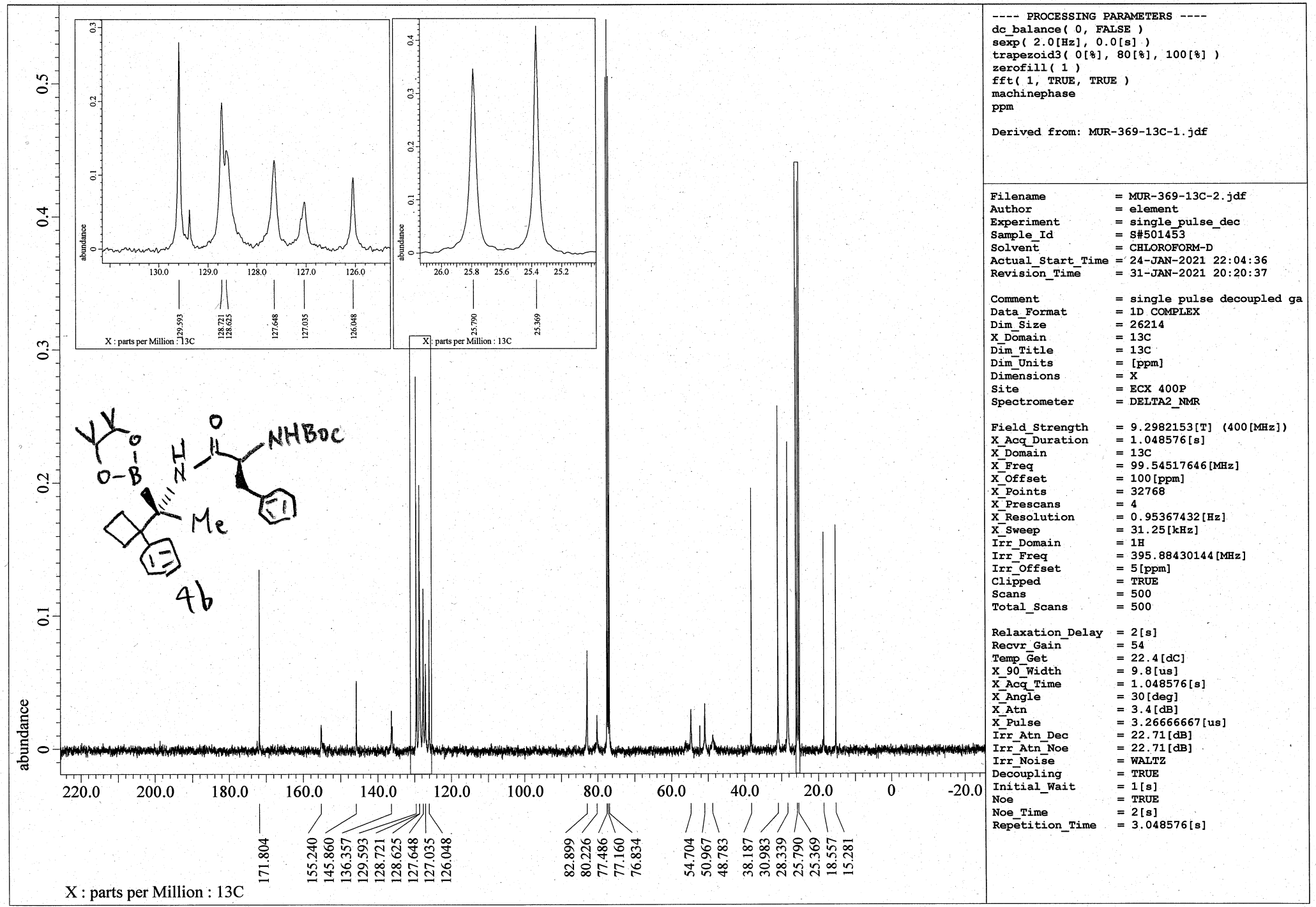

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: MUR-306-11B-1.jdf
```

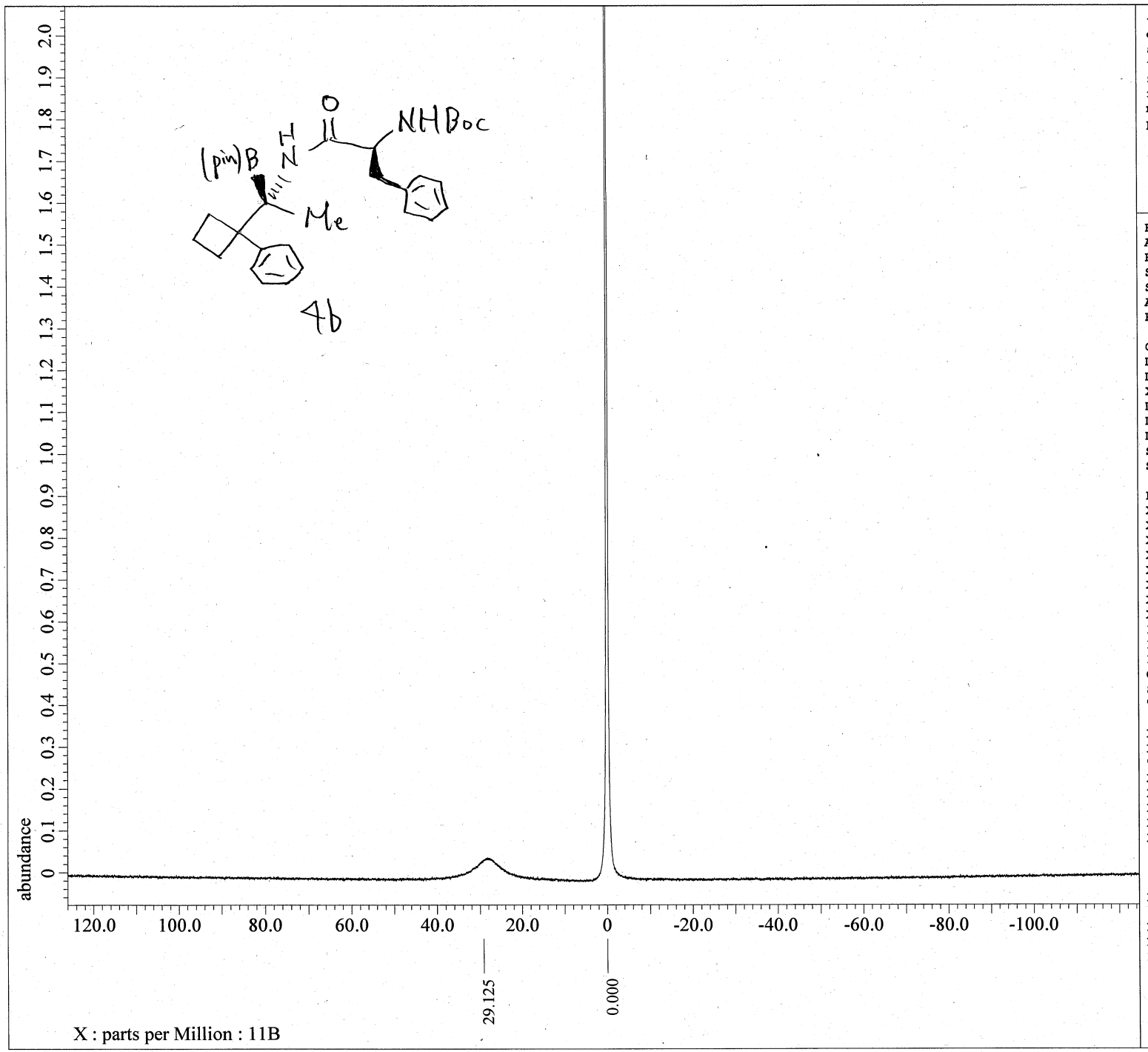
```
Filename            = MUR-306-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#499105
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  4-MAR-2021 21:59:45
Revision_Time       =  5-MAR-2021 09:24:44

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = TRUE
Scans               = 1000
Total_Scans         = 1000

Relaxation_Delay    = 2[s]
Recvr_Gain          = 56
Temp_Get            = 20.1[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[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

Derived from: MUR-369-proton-1.jdf
```

Filename	= MUR-369-proton-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#467896
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-JAN-2021 21:09:17
Revision_Time	= 25-JAN-2021 14:09:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 2.20725248[s]
X_Domain	= 1H
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 38
Temp_Get	= 21.5[dC]
X_90_Width	= 12.6[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 6.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.20725248[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
Derived from: MUR-369-13C-1.jdf
Filename = MUR-369-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#501453
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-JAN-2021 22:04:36
Revision_Time = 31-JAN-2021 20:20:37
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 500
Total_Scans = 500
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.4[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[s]
abundance
X : parts per Million : 13C
171.804
155.240
145.860
136.357
129.593
128.721
128.625
127.648
127.035
126.048
82.899
80.226
77.486
77.160
76.834
54.704
50.967
48.783
38.187
30.983
28.339
25.790
25.369
18.557
15.281
NHBoc
Me
4b




```
---- 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:: MUR-369-11B-1.jdf
```

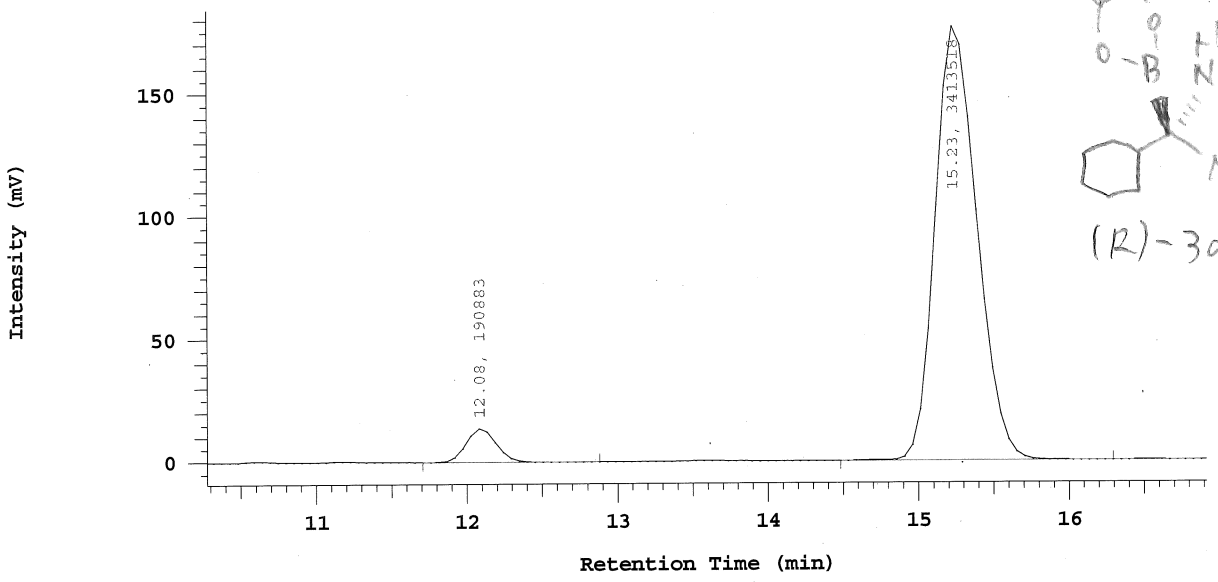
```
Filename            = MUR-369-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#603971
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  4-MAR-2021 00:54:02
Revision_Time       =  5-MAR-2021 09:25:14

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 284
Total_Scans         = 284

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20.2[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[us]
Irr_Atn_Dec         = 22.71[dB]
Irr_Atn_Noe         = 22.71[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.82313216[s]
```

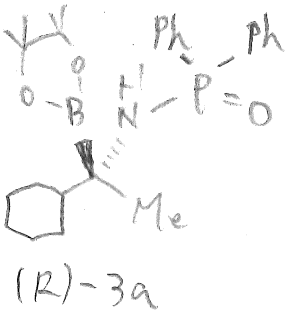
D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2021/01/06 16:13
Reported Date and Time: 2021/01/06 18:55
Processed Date and Time: 2021/01/06 18:55
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3131\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3131
Application(data): Isocratic HPLC
Vial Number: 142
Sample Name: MUR-363-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1





(R)-3a

Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	12.08	190883	5.296
2	15.23	3413518	94.704
		3604401	100.000

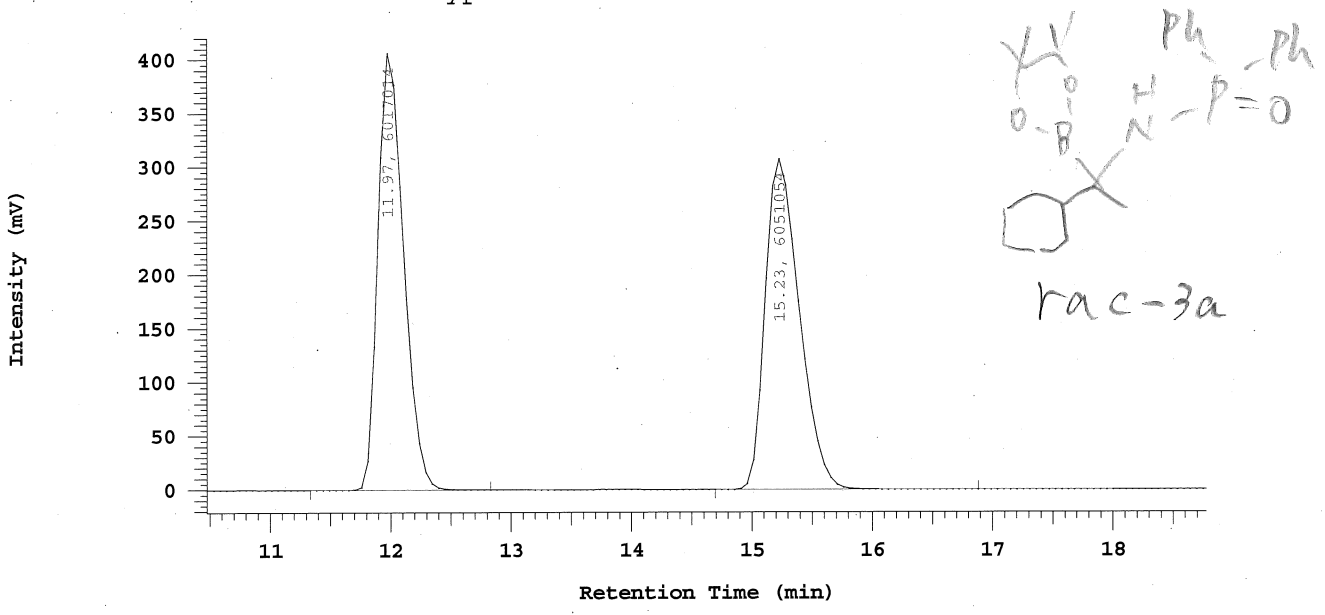
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2021/01/06 17:10
Reported Date and Time: 2021/01/06 18:56
Processed Date and Time: 2021/01/06 18:56
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3132\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3132
Application(data): Isocratic HPLC
Vial Number: 143
Sample Name: MUR-3a-rac
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	11.97	6017014	49.859
2	15.23	6051054	50.141
		12068068	100.000

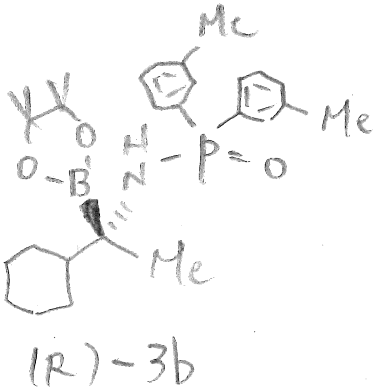
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

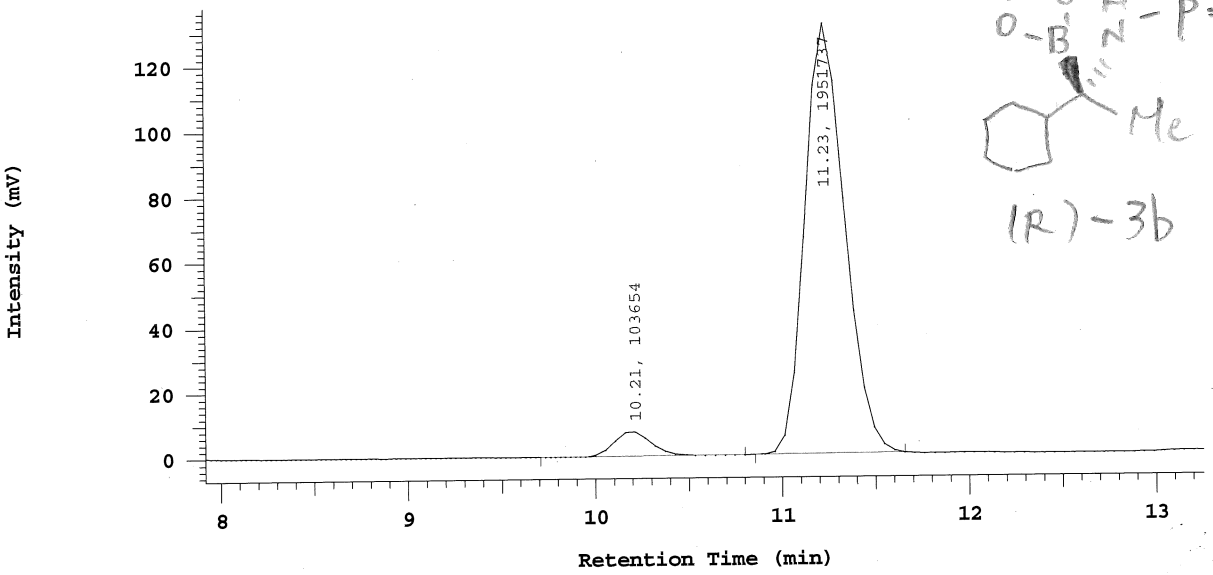
Analyzed Date and Time: 2020/04/15 15:22
Reported Date and Time: 2020/04/15 16:08
Processed Date and Time: 2020/04/15 16:07
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\2970\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Application(data): Isocratic HPLC
Sample Name: MUR-210-L22-OZ3-10%
Injection from this vial: 1 of 1
Sample Description:

Series: 2970
Vial Number: 145
Vial Type: UNK
Volume: 10.0 ul



Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	10.21	103654	5.043
2	11.23	1951737	94.957
		2055391	100.000

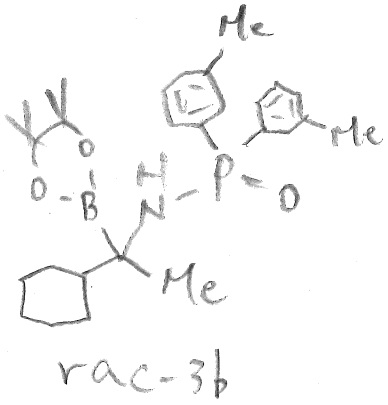
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/04/15 13:41
Reported Date and Time: 2020/04/15 15:24
Processed Date and Time: 2020/04/15 15:23
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\2969\
Processing Method: 10/90 iPrOH/Hexane

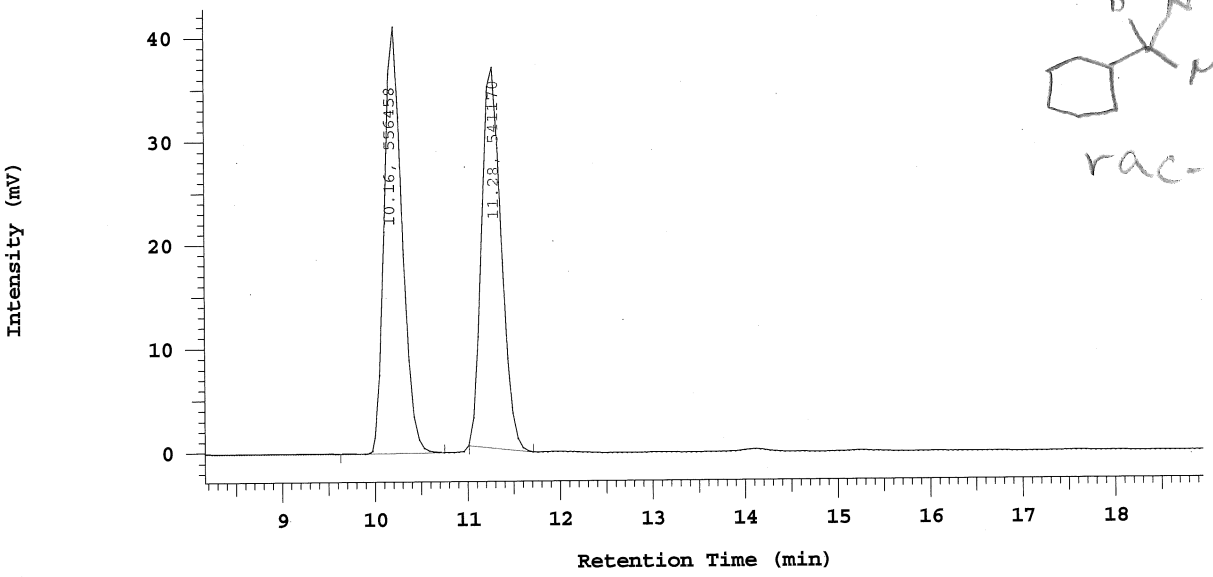
System (acquisition): Sys 1
Application(data): Isocratic HPLC
Sample Name: MUR-211-rac-OZ3-10%
Injection from this vial: 1 of 1
Sample Description:

Series: 2969
Vial Number: 144
Vial Type: UNK
Volume: 10.0 ul



rac-3b

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	10.16	556458	50.696
2	11.28	541170	49.304
		1097628	100.000

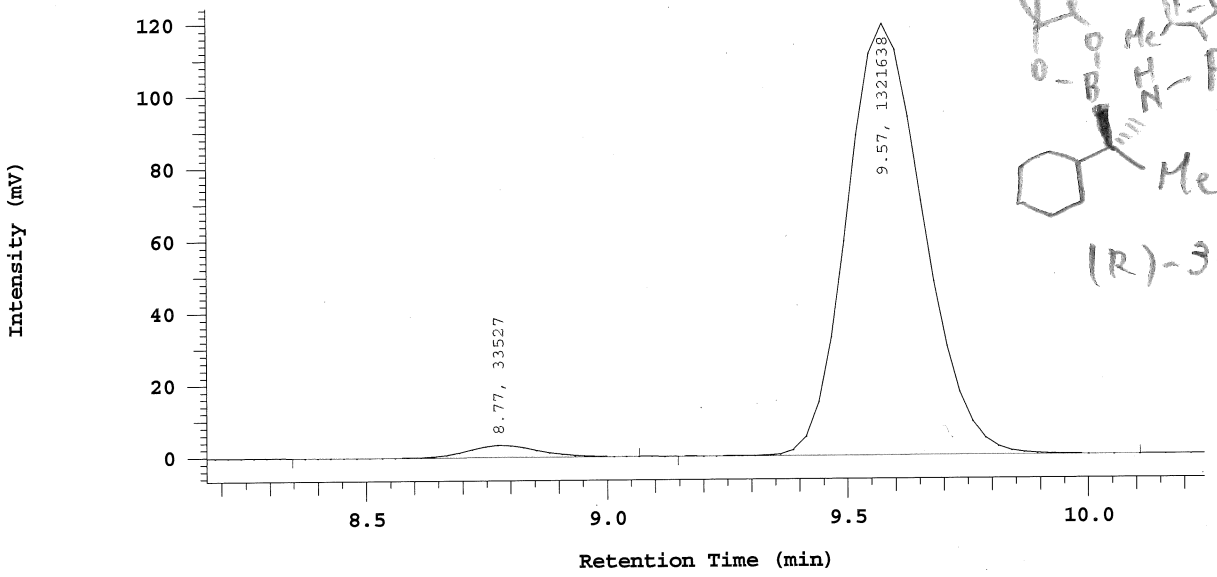
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/11/22 14:47
Reported Date and Time: 2020/11/22 17:25
Processed Date and Time: 2020/11/22 16:54
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3104\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3104
Application(data): Isocratic HPLC
Vial Number: 149
Sample Name: MUR-145-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	8.77	33527	2.474
2	9.57	1321638	97.526
		1355165	100.000

Peak rejection level: 0

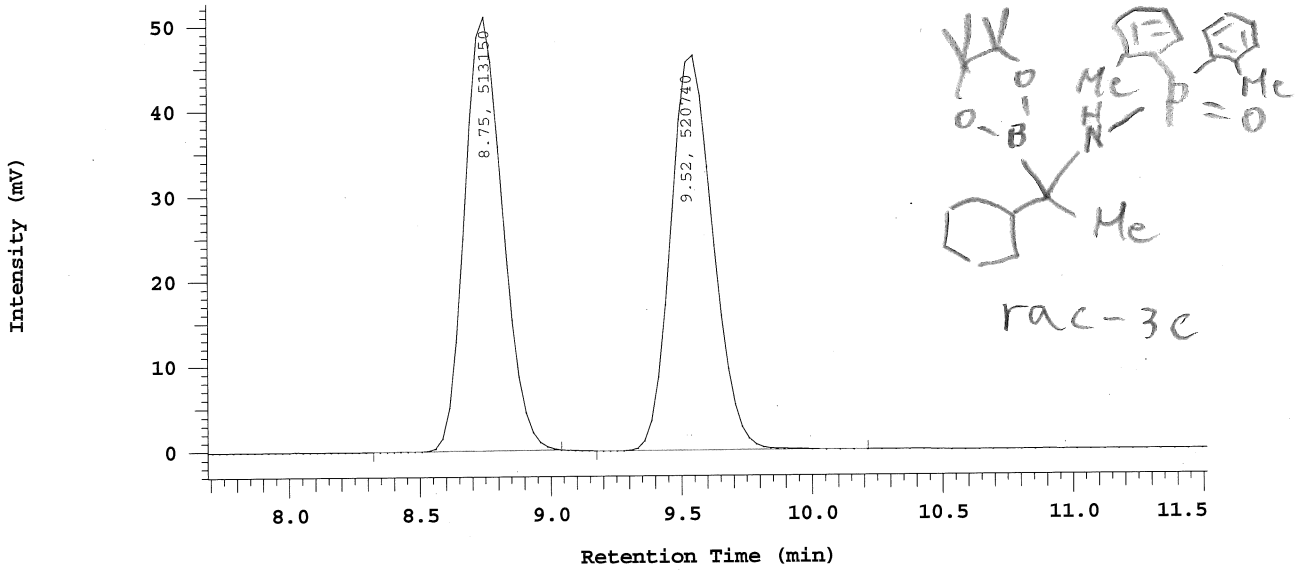
D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/11/22 18:28
Reported Date and Time: 2020/11/24 09:29
Processed Date and Time: 2020/11/24 09:28
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3105\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Application(data): Isocratic HPLC
Sample Name: MUR-1c-rac
Injection from this vial: 1 of 1
Sample Description:

Series: 3105
Vial Number: 150
Vial Type: UNK
Volume: 10.0 ul

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

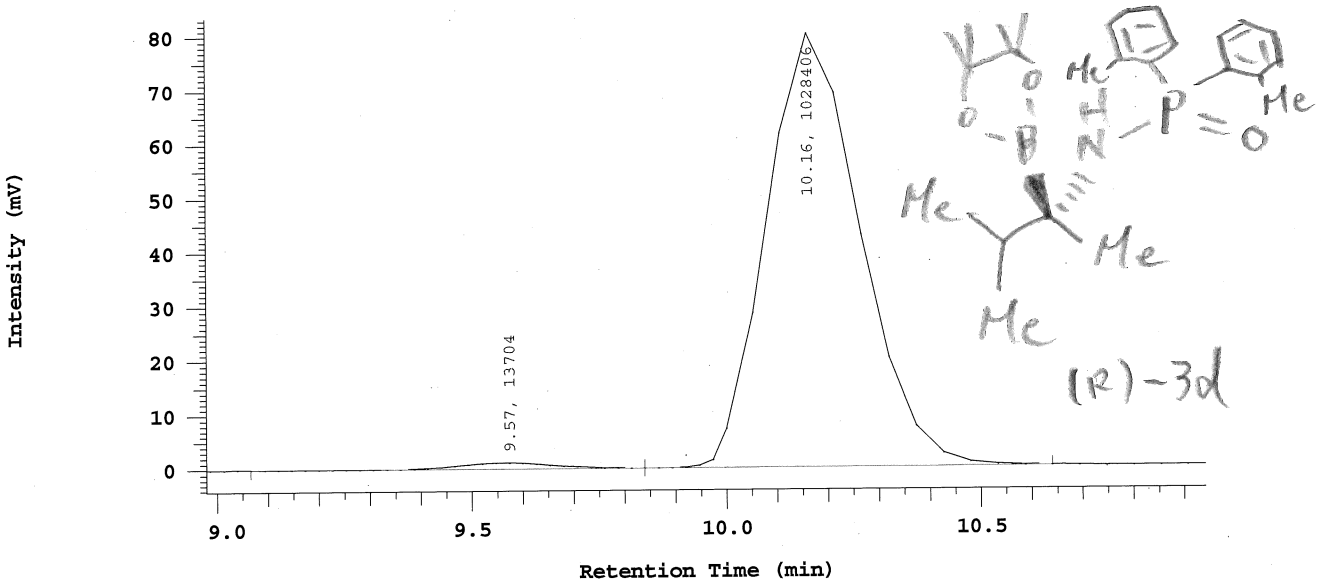
No.	RT	Area	Area %
1	8.75	513150	49.633
2	9.52	520740	50.367
		1033890	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2019/12/21 12:00
Reported Date and Time: 2019/12/21 13:35
Processed Date and Time: 2019/12/21 13:35
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\2939\
Processing Method: 10/90 iPrOH/Hexane
System (acquisition): Sys 1
Series: 2939
Application(data): Isocratic HPLC
Vial Number: 143
Sample Name: MUR-146-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1

Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	9.57	13704	1.315
2	10.16	1028406	98.685
		1042110	100.000

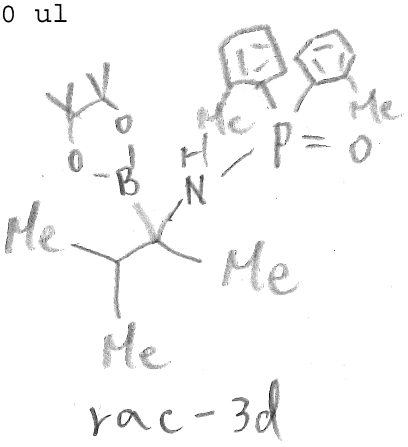
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2019/12/21 13:42
Reported Date and Time: 2020/01/23 19:58
Processed Date and Time: 2020/01/23 19:58
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\2940\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Application(data): Isocratic HPLC
Sample Name: MUR-rac 147
Injection from this vial: 1 of 1
Sample Description:

Series: 2940
Vial Number: 144
Vial Type: UNK
Volume: 10.0 ul



Chrom Type: HPLC Channel : 1

Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

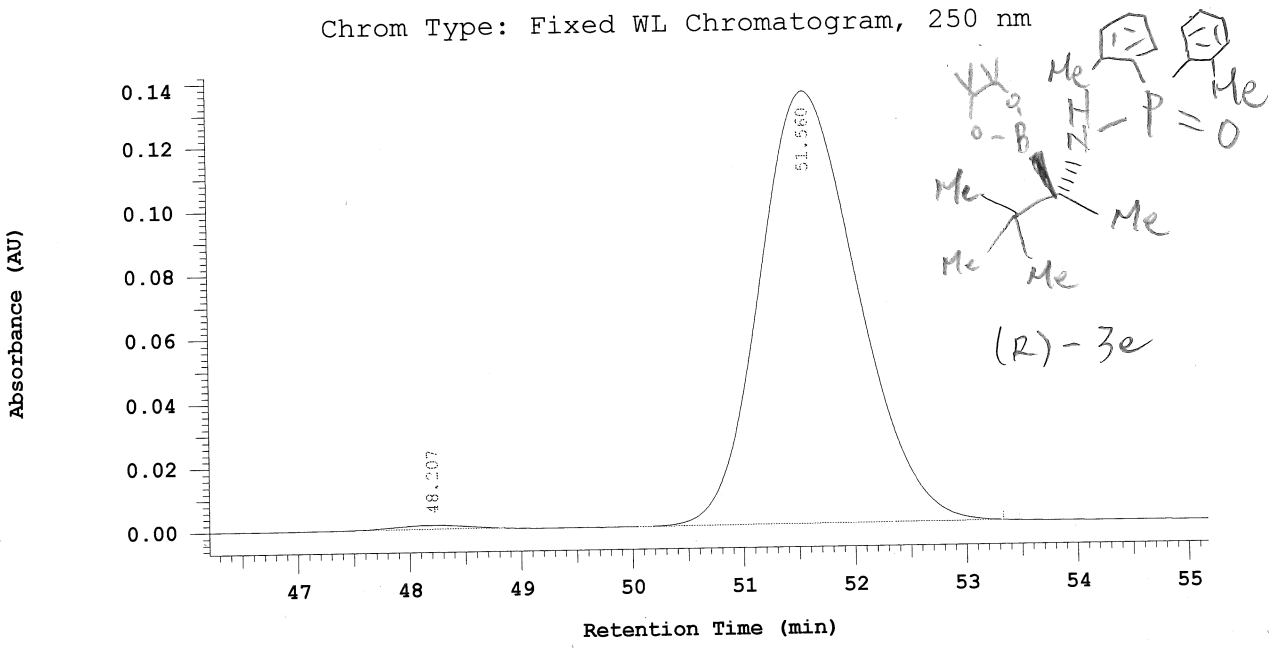
No.	RT	Area	Area %
1	9.55	260109	49.572
2	10.16	264602	50.428
		524711	100.000

Peak rejection level: 0

Chromaster System Manager Report

Analyzed Date and Time: 2019/12/24 00:17
Reported Date and Time: 2019/12/24 09:55:33
Processed Date and Time: 2019/12/24 09:55
Data Path: C:\WIN32APP\CHROMASTER\MUR\DATA\0002\
Processing Method: column1(IA-3)
System (acquisition): Sys 1
Application(data): MUR
Sample Name: MUR-148-IA-8%
Injection from this vial: 1 of 1
Sample Description:
Series: 0002
Vial Number: 10
Vial Type: UNK
Volume: 10.0 ul

Chrom Type: Fixed WL Chromatogram, 250 nm



Processing Method: column1(IA-3)
Method Developer:
Pump 1: 5110
Pump 1 Solvent A: hexane
Pump 1 Solvent B: 2-propanol
Pump 1 Solvent C:
Pump 1 Solvent D:
Method Description:

Chrom Type: Fixed WL Chromatogram, 250 nm

Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Conc 1	BC
1	48.207	25084	0.607	BB
2	51.560	4108822	99.393	BB
		4133906	100.000	

Peak rejection level: 0

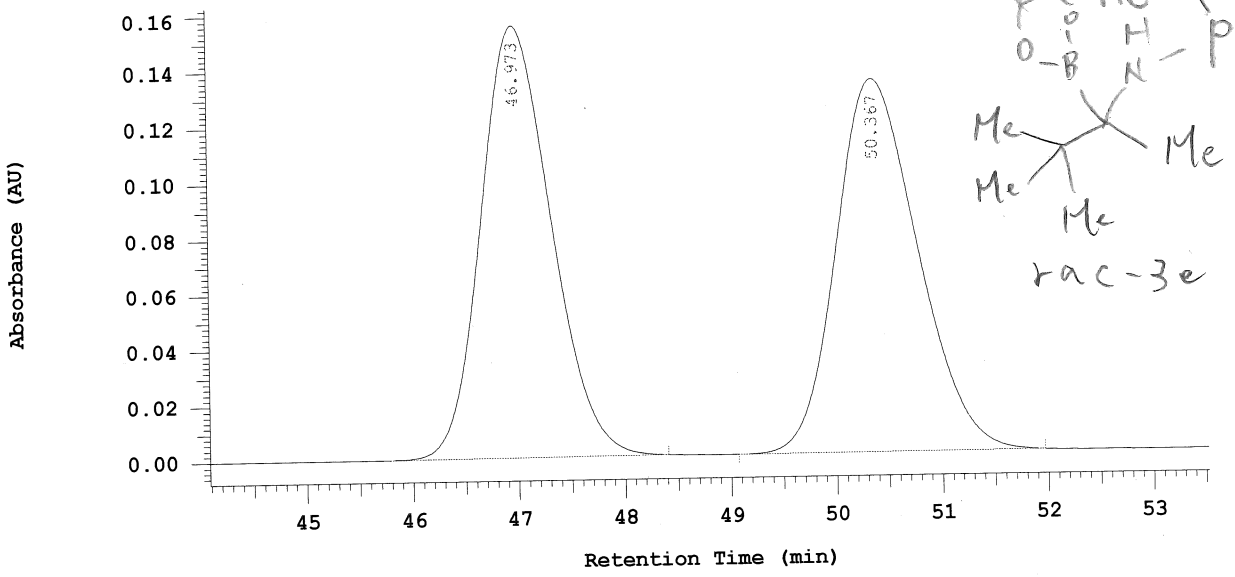
Chromaster System Manager Report

Analyzed Date and Time: 2019/12/23 22:05
Reported Date and Time: 2019/12/24 09:54:25
Processed Date and Time: 2019/12/24 09:53
Data Path: C:\WIN32APP\CHROMASTER\MUR\DATA\0001\
Processing Method: column1(IA-3)

System (acquisition): Sys 1
Application(data): MUR
Sample Name: MUR-149-IA-8%
Injection from this vial: 1 of 1
Sample Description:

Series: 0001
Vial Number: 9
Vial Type: UNK
Volume: 10.0 ul

Chrom Type: Fixed WL Chromatogram, 250 nm



Processing Method: column1(IA-3)
Method Developer:
Pump 1: 5110
Pump 1 Solvent A: hexane
Pump 1 Solvent B: 2-propanol
Pump 1 Solvent C:
Pump 1 Solvent D:
Method Description:

Chrom Type: Fixed WL Chromatogram, 250 nm

Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Conc 1	BC
1	46.973	3579983	49.938	BB
2	50.367	3588904	50.062	BB
		7168887	100.000	

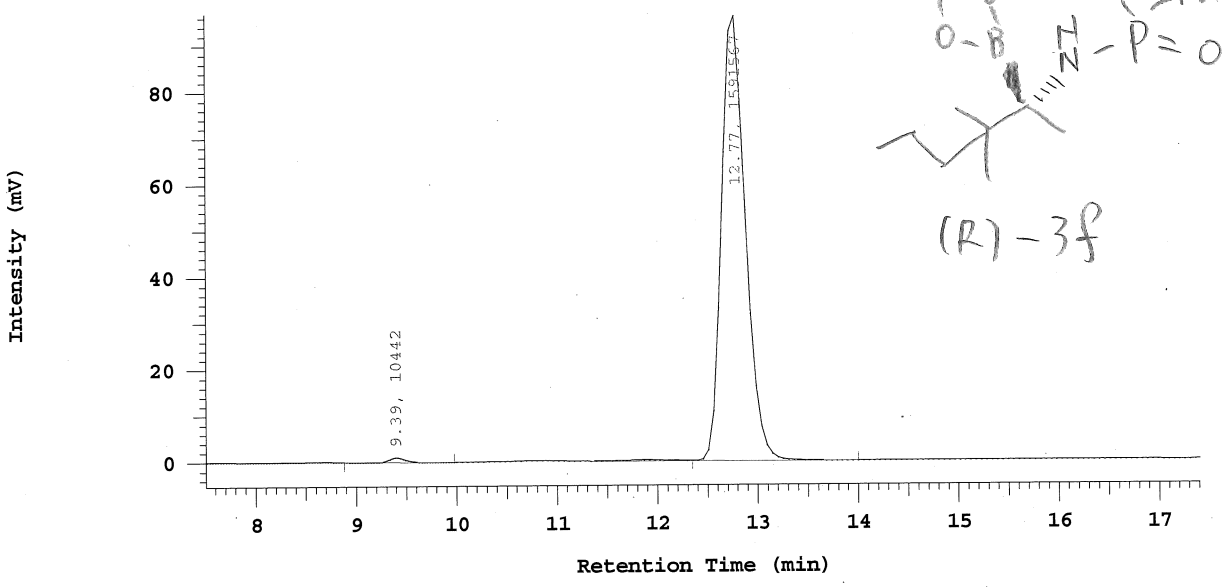
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/06/24 14:22
Reported Date and Time: 2020/06/24 15:43
Processed Date and Time: 2020/06/24 15:43
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3017\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3017
Application(data): Isocratic HPLC
Vial Number: 142
Sample Name: MUR-249-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

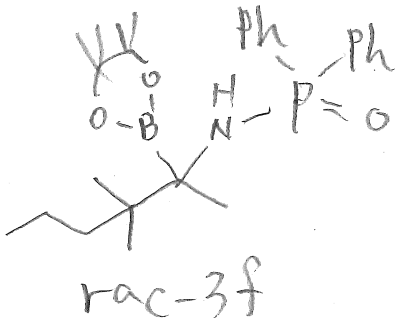
No.	RT	Area	Area %
1	9.39	10442	0.652
2	12.77	1591567	99.348
		1602009	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

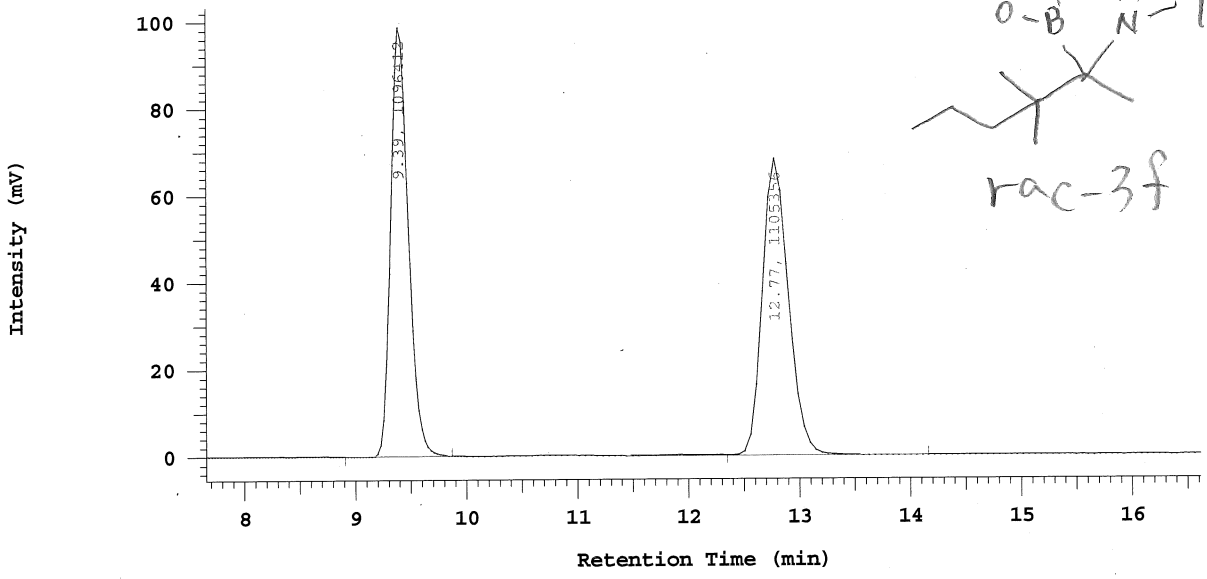
Analyzed Date and Time: 2020/06/24 15:29
Reported Date and Time: 2020/06/24 17:13
Processed Date and Time: 2020/06/24 17:12
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3018\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3018
Application(data): Isocratic HPLC
Vial Number: 143
Sample Name: MUR-247-rac-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:



rac-3f

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

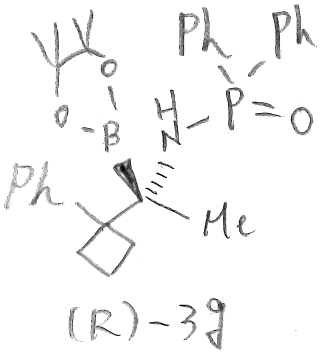
No.	RT	Area	Area %
1	9.39	1096412	49.797
2	12.77	1105356	50.203
		2201768	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

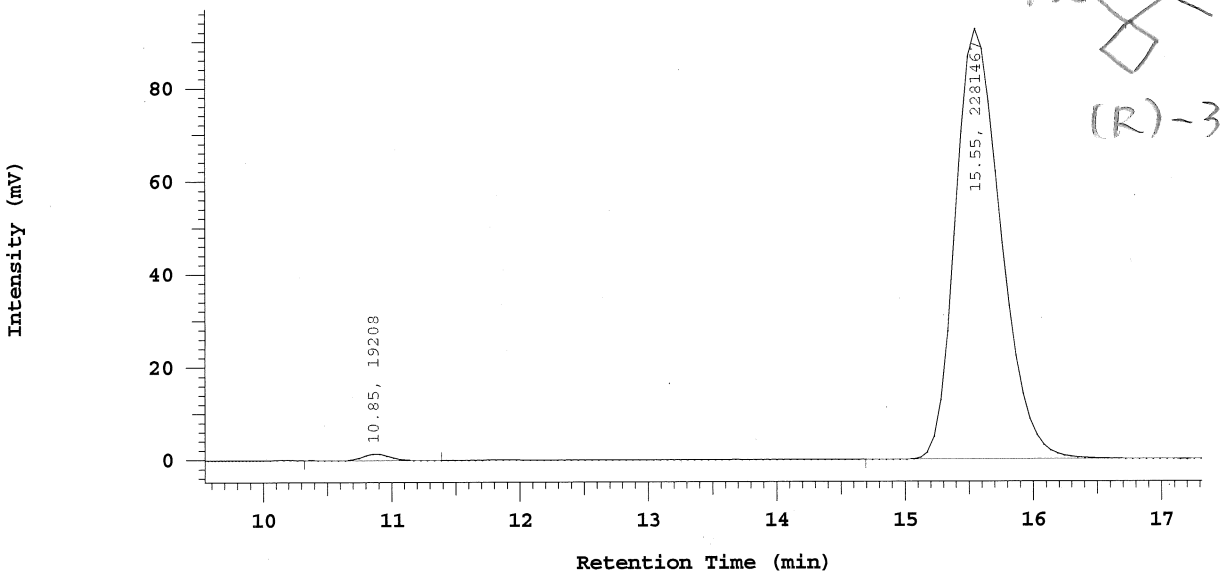
Analyzed Date and Time: 2020/07/04 17:44
Reported Date and Time: 2020/09/02 20:47
Processed Date and Time: 2020/09/02 20:47
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3030\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3030
Application(data): Isocratic HPLC
Vial Number: 142
Sample Name: MUR-265-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:



(R)-3g

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	10.85	19208	0.835
2	15.55	2281467	99.165
		2300675	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/07/04 16:52 Reported Date and Time: 2020/09/02 20:47

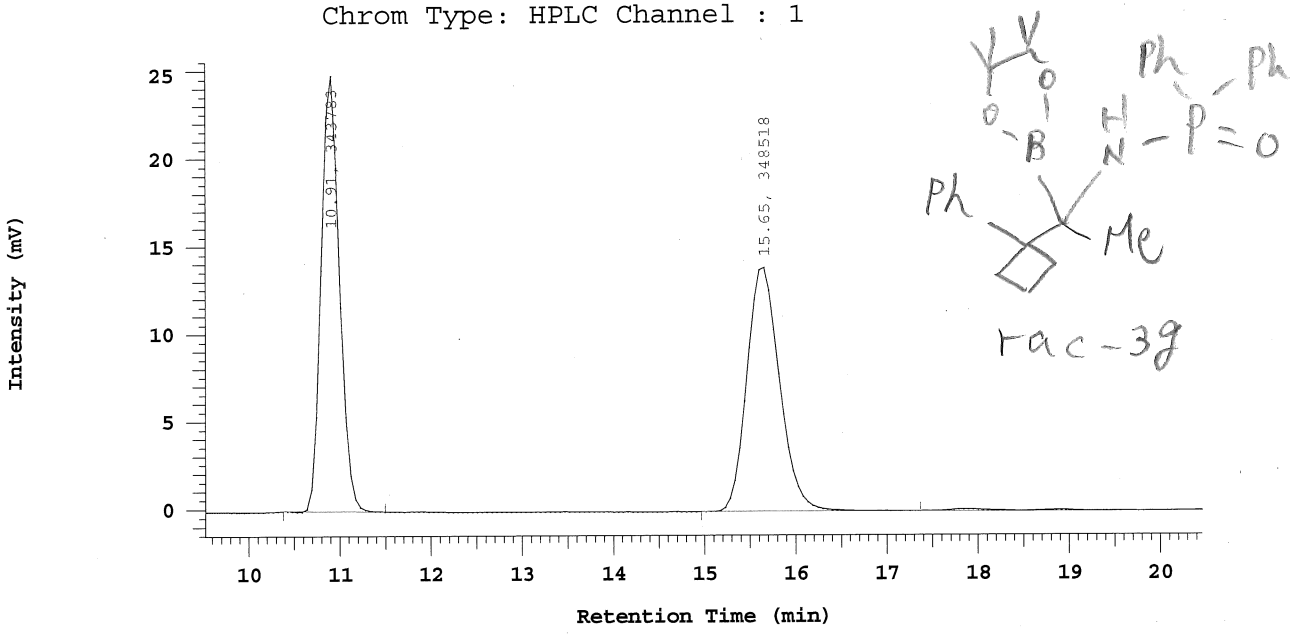
Processed Date and Time: 2020/09/02 20:47

Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3029\

Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1 Series: 3029
Application(data): Isocratic HPLC Vial Number: 141
Sample Name: MUR-262-rac-OZ3-10% Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2 Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	10.91	343783	49.658
2	15.65	348518	50.342
		692301	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/08/03 16:39 Reported Date and Time: 2020/08/03 18:22

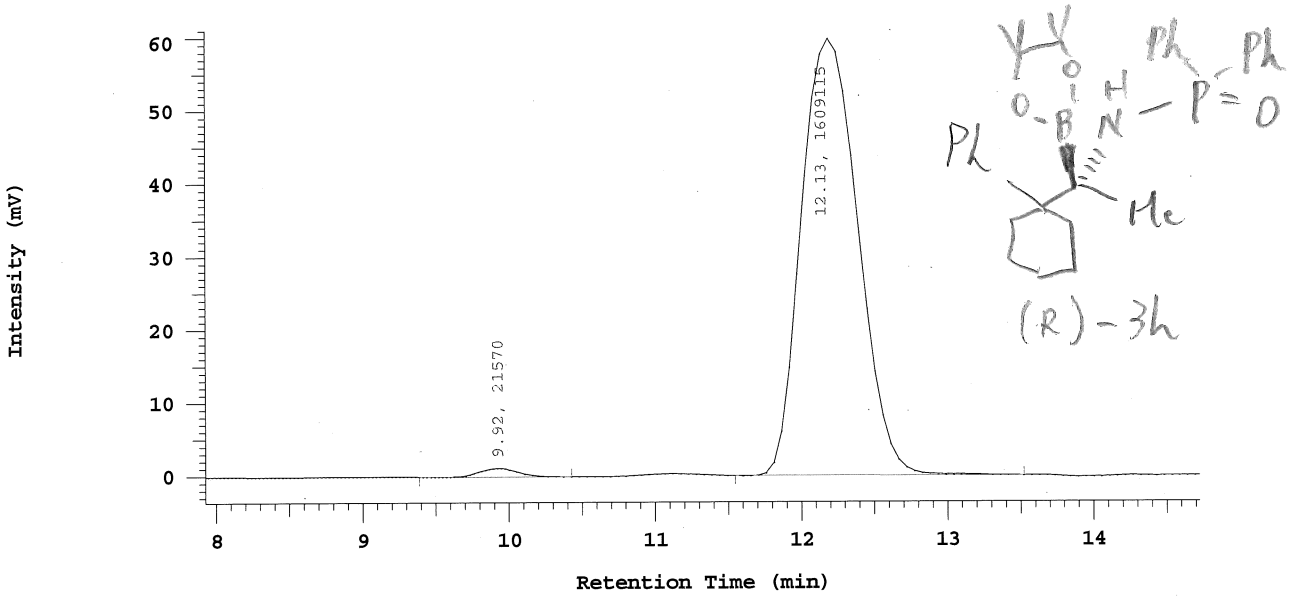
Processed Date and Time: 2020/08/03 18:21

Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3040\

Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1 Series: 3040
Application(data): Isocratic HPLC Vial Number: 142
Sample Name: MUR-279-L22-OZ3-10% Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2 Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	9.92	21570	1.323
2	12.13	1609115	98.677
		1630685	100.000

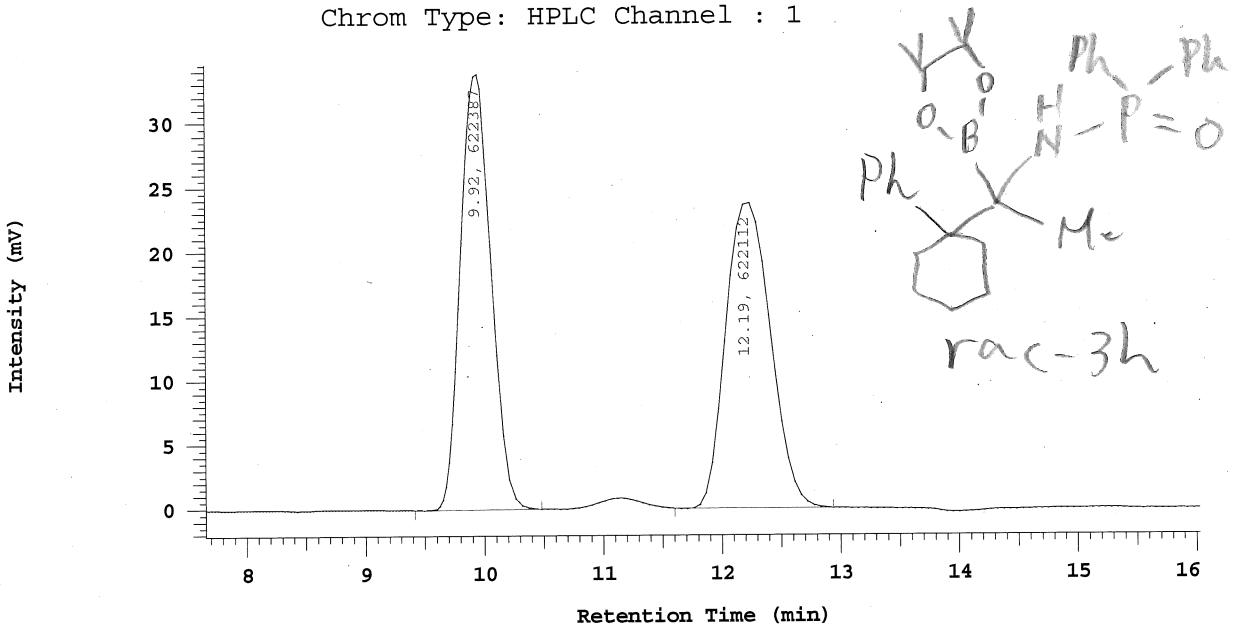
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/08/03 15:27
Reported Date and Time: 2020/08/03 16:48
Processed Date and Time: 2020/08/03 16:48
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3039\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3039
Application(data): Isocratic HPLC
Vial Number: 141
Sample Name: MUR-280-rac-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	9.92	622387	50.011
2	12.19	622112	49.989
		1244499	100.000

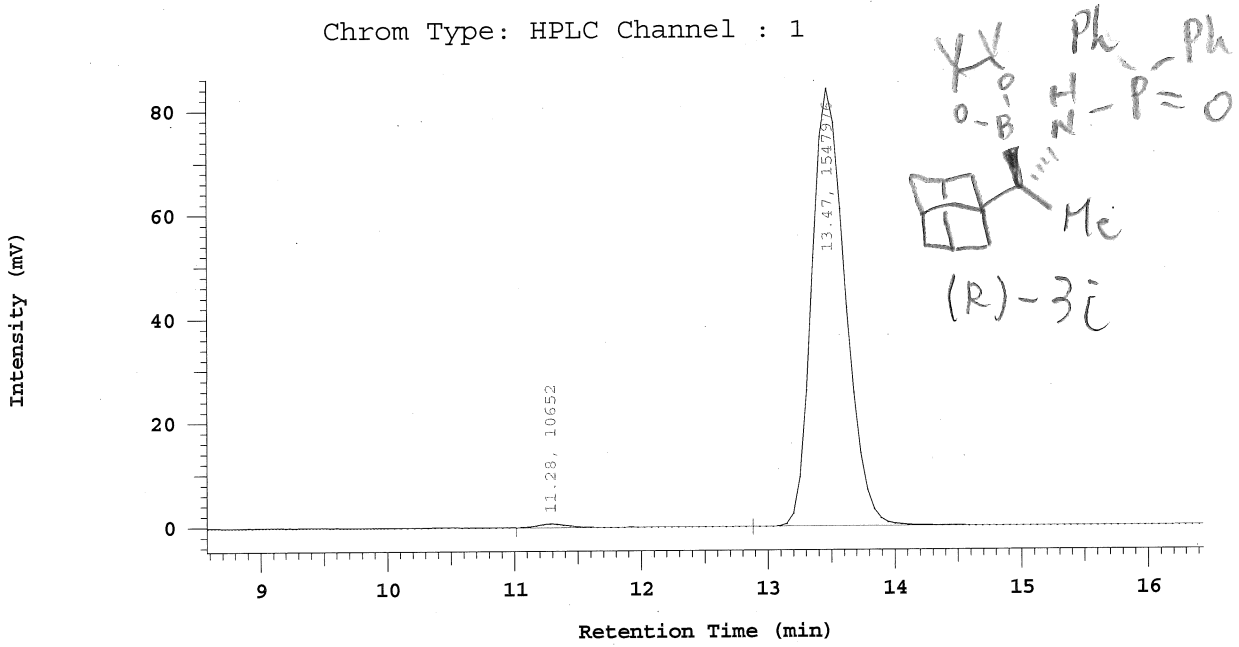
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/06/29 15:44
Reported Date and Time: 2020/06/29 17:39
Processed Date and Time: 2020/06/29 17:39
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3025\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3025
Application(data): Isocratic HPLC
Vial Number: 141
Sample Name: MUR-260-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

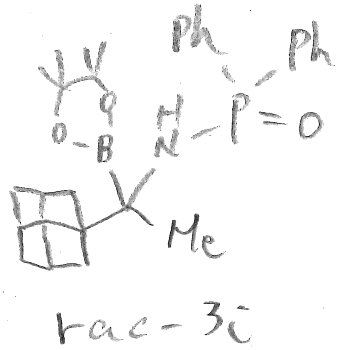
Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	11.28	10652	0.683
2	13.47	1547976	99.317
		1558628	100.000

Peak rejection level: 0

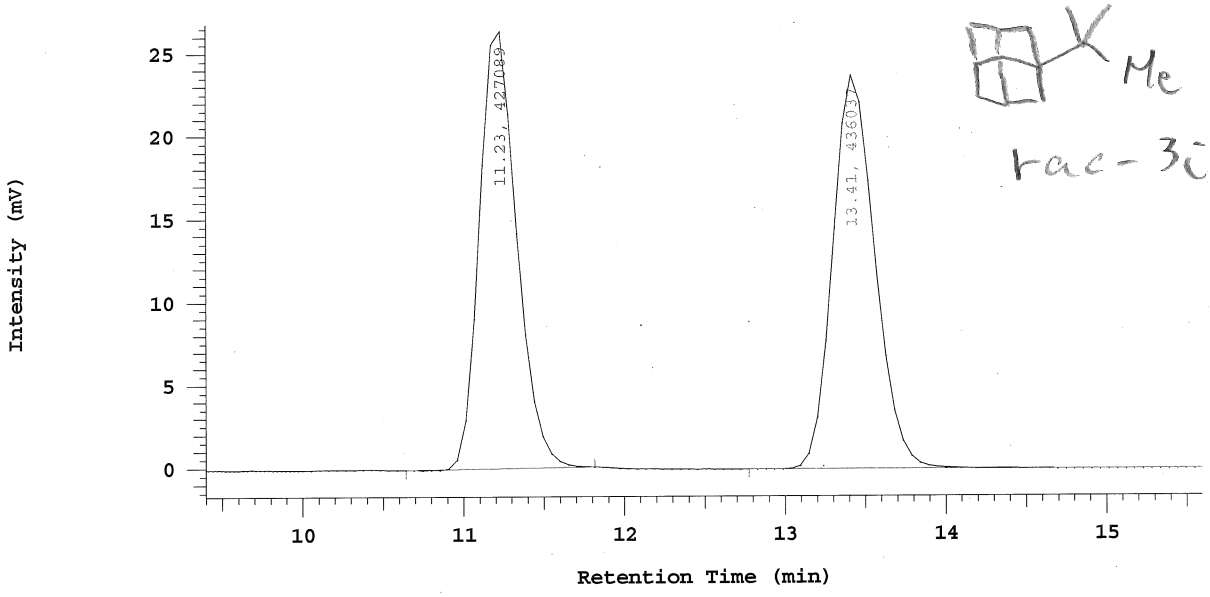
D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/06/29 17:26
Reported Date and Time: 2020/06/29 18:55
Processed Date and Time: 2020/06/29 18:55
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3026\
Processing Method: 10/90 iPrOH/Hexane
System (acquisition): Sys 1
Series: 3026
Application(data): Isocratic HPLC
Vial Number: 142
Sample Name: MUR-255-rac-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:



rac-3i

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	11.23	427089	49.482
2	13.41	436037	50.518
		863126	100.000

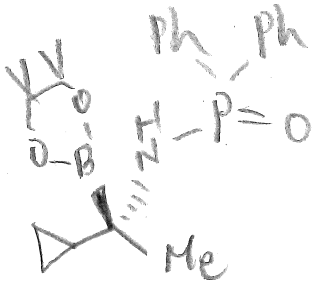
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/06/13 13:10
Reported Date and Time: 2020/06/13 14:33
Processed Date and Time: 2020/06/13 14:33
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3003\
Processing Method: 10/90 iPrOH/Hexane

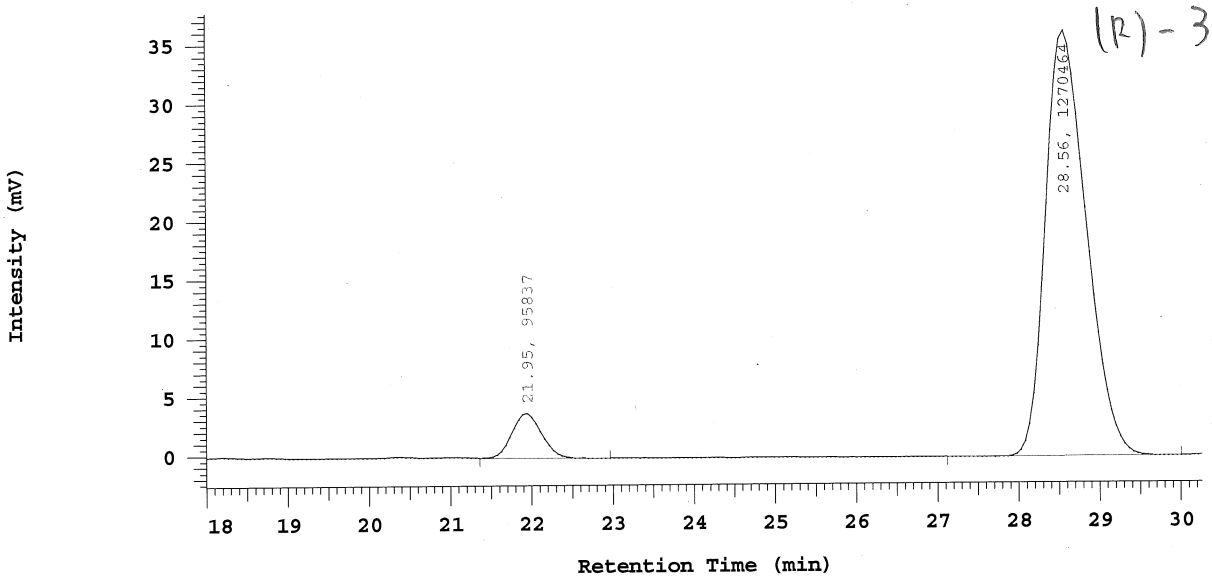
System (acquisition): Sys 1
Application(data): Isocratic HPLC
Sample Name: MUR-232-OZ3-10%
Injection from this vial: 1 of 1
Sample Description:

Series: 3003
Vial Number: 141
Vial Type: UNK
Volume: 10.0 ul



(R)-3j

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	21.95	95837	7.014
2	28.56	1270464	92.986
		1366301	100.000

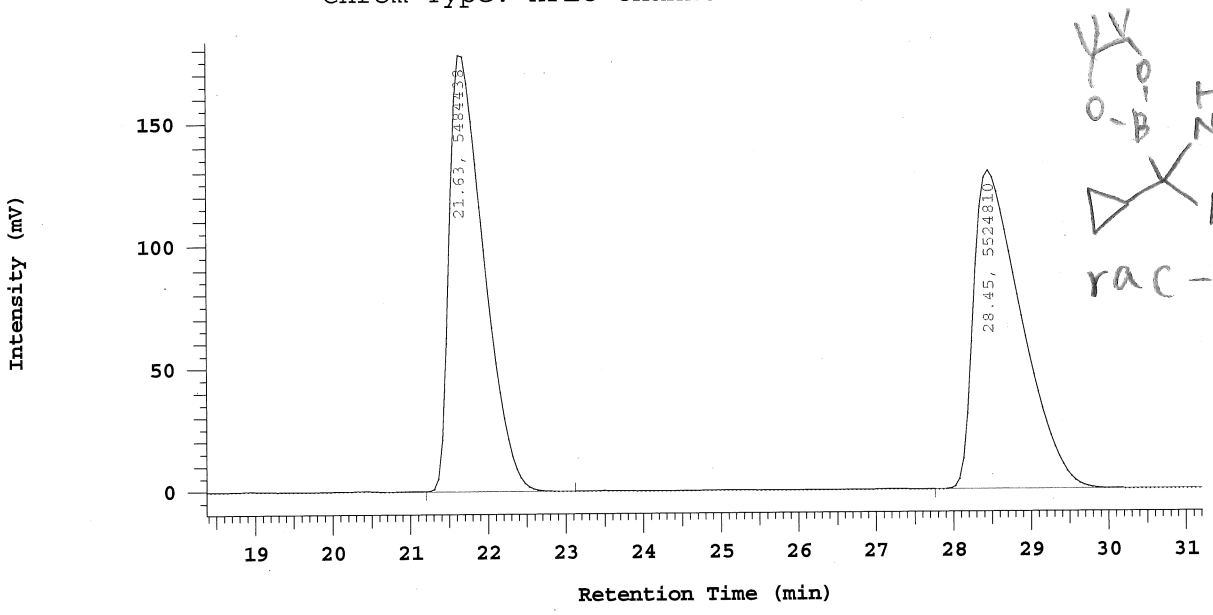
Peak rejection level: 0

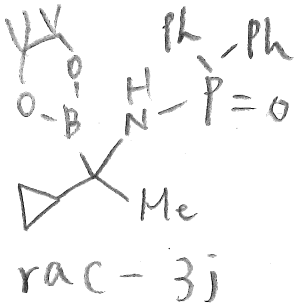
D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/06/13 14:32
Reported Date and Time: 2020/06/13 16:51
Processed Date and Time: 2020/06/13 16:51
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3004\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3004
Application(data): Isocratic HPLC
Vial Number: 142
Sample Name: MUR-231-rac-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1





Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	21.63	5484438	49.817
2	28.45	5524810	50.183
		11009248	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/07/02 16:04 Reported Date and Time: 2020/07/02 16:42

Processed Date and Time: 2020/07/02 16:40

Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3027\

Processing Method: 10/90 iPrOH/Hexane

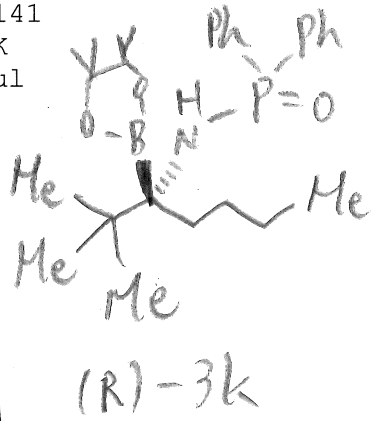
System (acquisition): Sys 1 Series: 3027

Application(data): Isocratic HPLC Vial Number: 141

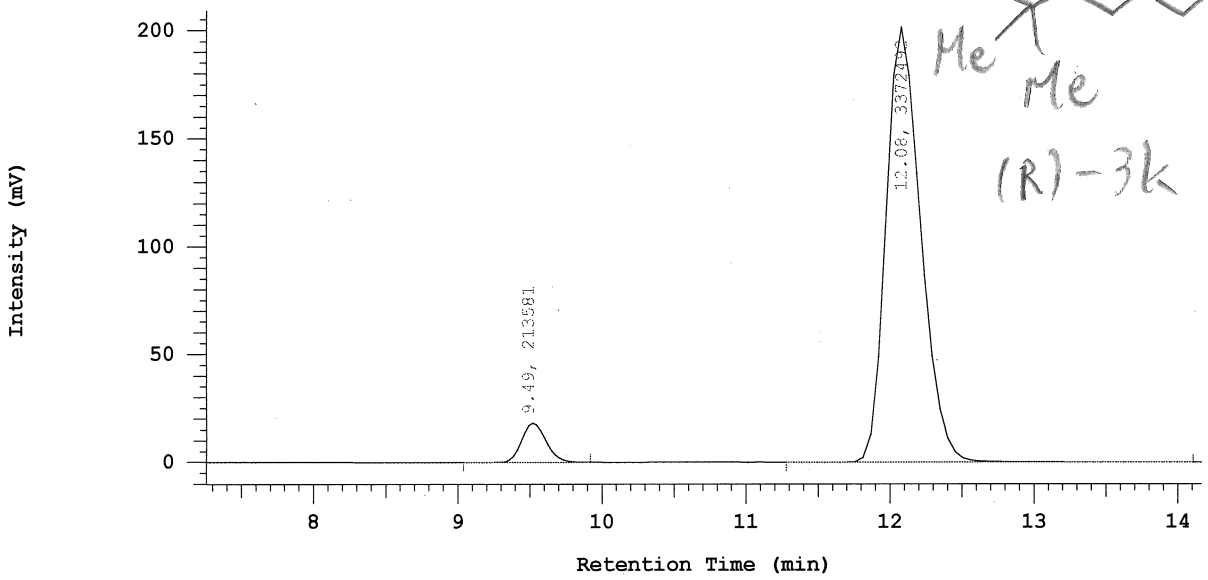
Sample Name: MUR-264-OZ3-10% Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:



Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane

Column Type: OD-H 2 Method Developer: Administrator

Pump A: L-2130

Pump A Solvent A: Hexane Pump A Solvent B: 10/90 iPrOH/Hexane

Pump A Solvent C: iPrOH Pump A Solvent D: iPrOH

Method Description:

Chrom Type: HPLC Channel : 1

Peak Quantitation: AREA

Calculation Method: AREA%

No.	RT	Area	Area %
1	9.49	213581	5.956
2	12.08	3372492	94.044
		3586073	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/07/02 16:46 Reported Date and Time: 2020/07/02 17:28

Processed Date and Time: 2020/07/02 17:28

Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3028\

Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1 Series: 3028

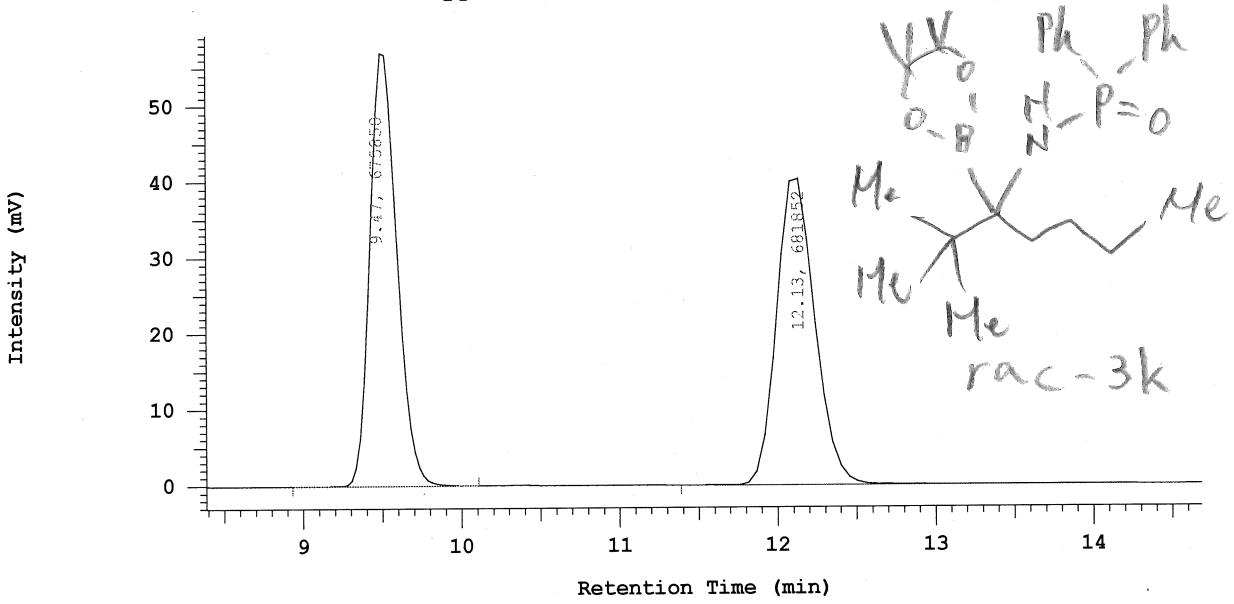
Application(data): Isocratic HPLC Vial Number: 142

Sample Name: MUR-263-rac-OZ3-10% Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane

Column Type: OD-H 2 Method Developer: Administrator

Pump A: L-2130

Pump A Solvent A: Hexane Pump A Solvent B: 10/90 iPrOH/Hexane

Pump A Solvent C: iPrOH Pump A Solvent D: iPrOH

Method Description:

Chrom Type: HPLC Channel : 1

Peak Quantitation: AREA

Calculation Method: AREA%

No.	RT	Area	Area %
1	9.47	675850	49.779
2	12.13	681852	50.221
		1357702	100.000

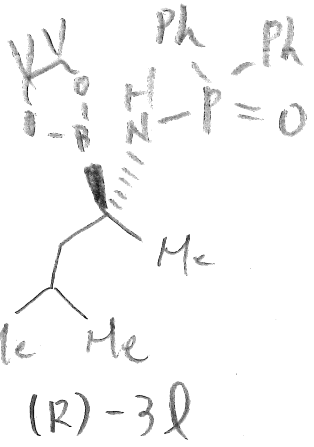
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/09/25 10:22
Reported Date and Time: 2020/09/25 11:06
Processed Date and Time: 2020/09/25 11:05
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3079\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Application(data): Isocratic HPLC
Sample Name: MUR-313-L22-OZ3-10%
Injection from this vial: 1 of 1
Sample Description:

Series: 3079
Vial Number: 145
Vial Type: UNK
Volume: 10.0 ul



Chrom Type: HPLC Channel : 1

Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	13.73	309747	5.941
2	17.52	4904361	94.059
		5214108	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/09/25 17:34 Reported Date and Time: 2020/09/25 19:57

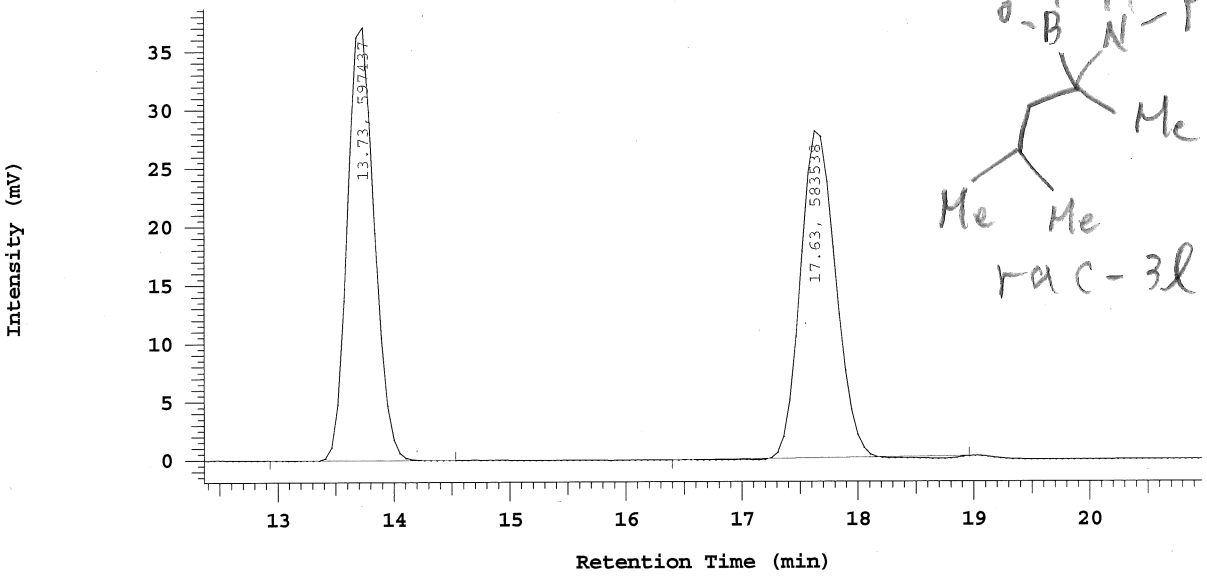
Processed Date and Time: 2020/09/25 19:57

Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3081\

Processing Method: 03/97 iPrOH/Hexane

System (acquisition): Sys 1 Series: 3081
Application(data): Isocratic HPLC Vial Number: 146
Sample Name: MUR-314-rac-OZ3-10% Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 10.0 ul
Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 03/97 iPrOH/Hexane
Column Type: OD-H 2 Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	13.73	597437	50.588
2	17.63	583538	49.412
		1180975	100.000

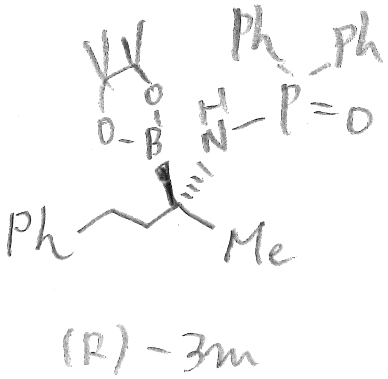
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2020/10/16 21:24
Reported Date and Time: 2020/10/16 23:15
Processed Date and Time: 2020/10/16 23:15
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3097\
Processing Method: 05/95 iPrOH/Hexane

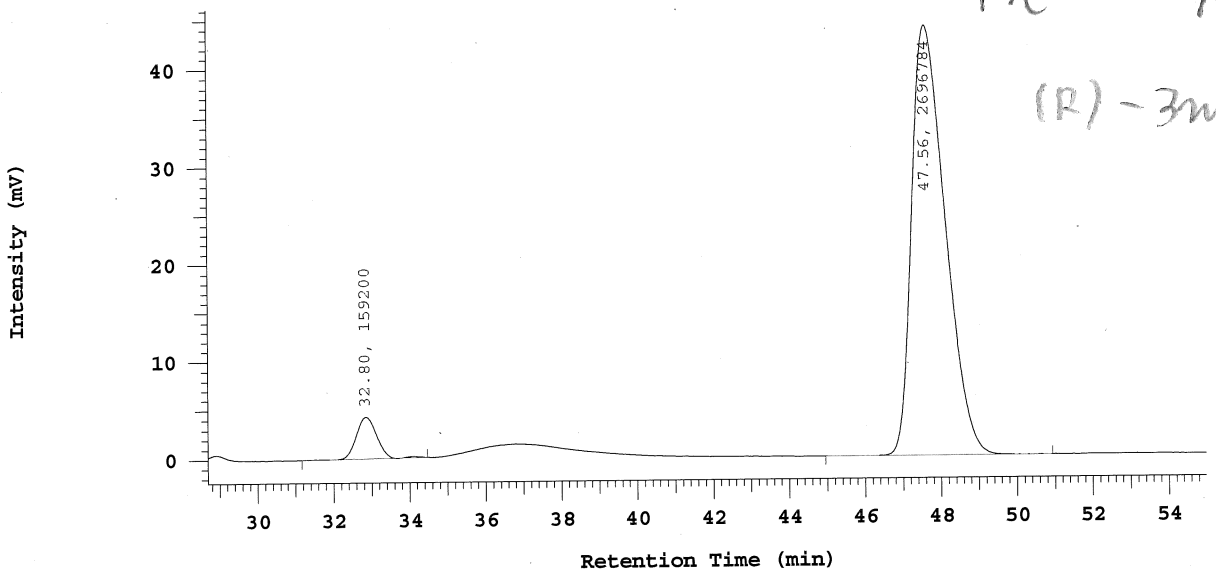
System (acquisition): Sys 1
Application(data): Isocratic HPLC
Sample Name: MUR-326-2-OZ3-5%
Injection from this vial: 1 of 1
Sample Description:

Series: 3097
Vial Number: 143
Vial Type: UNK
Volume: 10.0 ul



(R)-3m

Chrom Type: HPLC Channel : 1



Processing Method: 05/95 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	32.80	159200	5.574
2	47.56	2696784	94.426
		2855984	100.000

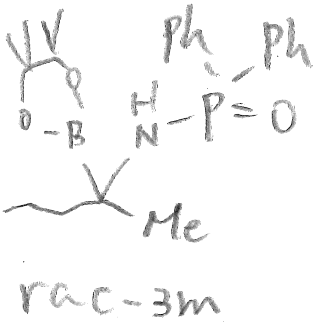
Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

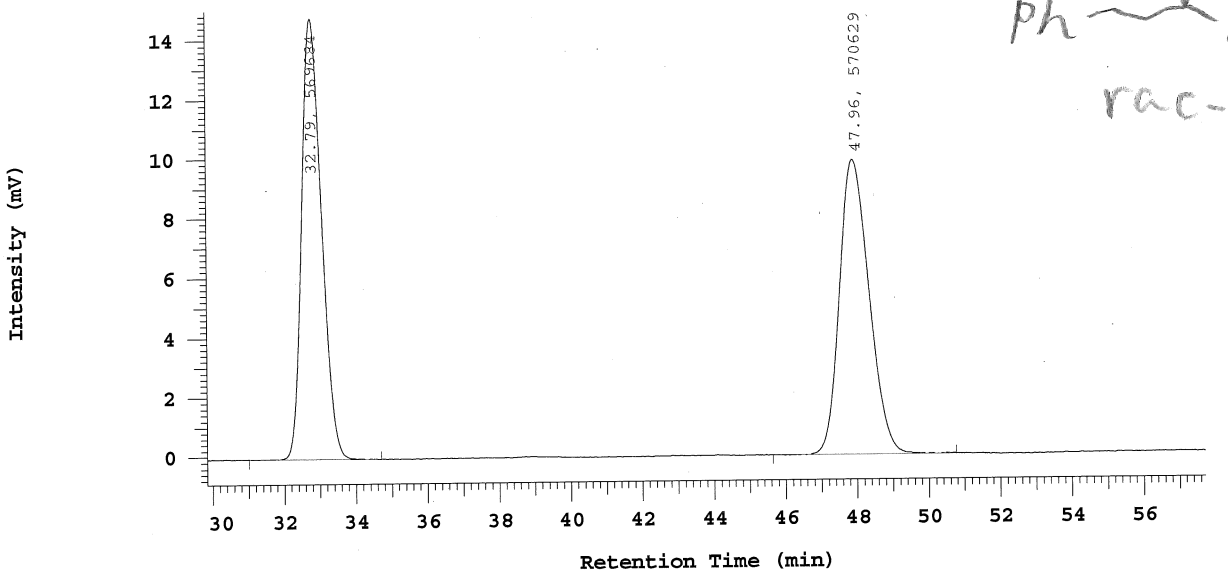
Analyzed Date and Time: 2020/10/16 22:56
Reported Date and Time: 2020/10/17 00:18
Processed Date and Time: 2020/10/17 00:18
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3098\
Processing Method: 05/95 iPrOH/Hexane

System (acquisition): Sys 1
Application(data): Isocratic HPLC
Sample Name: MUR-327-OZ3-10%
Injection from this vial: 1 of 1
Sample Description:

Series: 3098
Vial Number: 141
Vial Type: UNK
Volume: 10.0 ul



Chrom Type: HPLC Channel : 1



Processing Method: 05/95 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

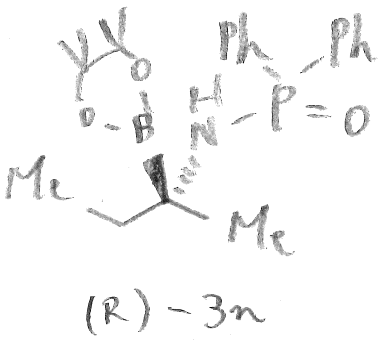
No.	RT	Area	Area %
1	32.79	569684	49.959
2	47.96	570629	50.041
		1140313	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

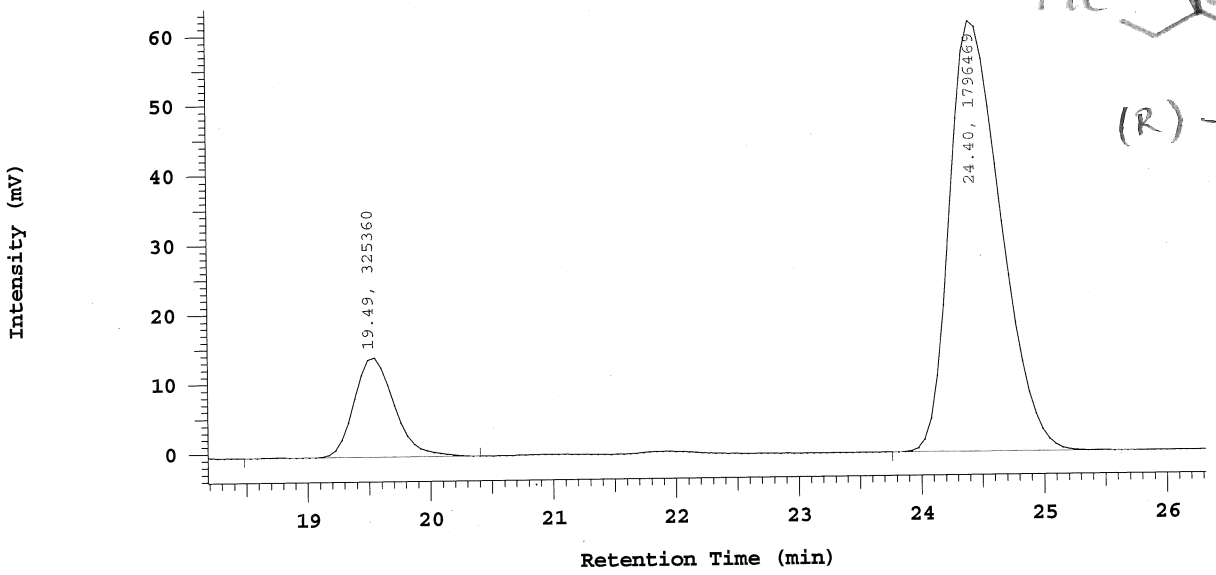
Analyzed Date and Time: 2020/10/31 18:04
Reported Date and Time: 2020/10/31 19:33
Processed Date and Time: 2020/10/31 19:33
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3102\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3102
Application(data): Isocratic HPLC
Vial Number: 148
Sample Name: MUR-333-rac-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:



(R)-3n

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1

Peak Quantitation: AREA
Calculation Method: AREA%

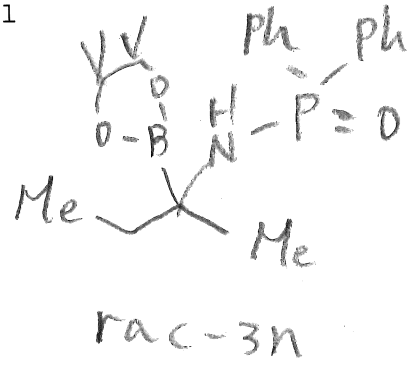
No.	RT	Area	Area %
1	19.49	325360	15.334
2	24.40	1796469	84.666
		2121829	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

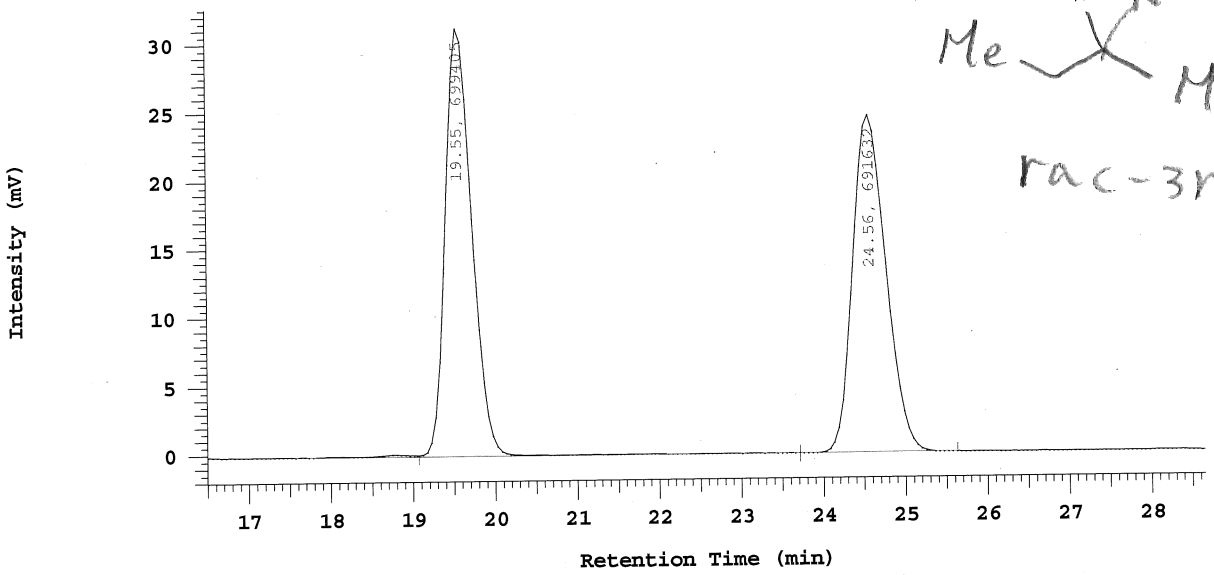
Analyzed Date and Time: 2020/10/31 15:25
Reported Date and Time: 2020/10/31 16:49
Processed Date and Time: 2020/10/31 16:48
Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\3101\
Processing Method: 10/90 iPrOH/Hexane

System (acquisition): Sys 1
Series: 3101
Application(data): Isocratic HPLC
Vial Number: 148
Sample Name: MUR-332-rac-OZ3-10%
Vial Type: UNK
Injection from this vial: 1 of 1
Volume: 10.0 ul
Sample Description:



rac-3n

Chrom Type: HPLC Channel : 1



Processing Method: 10/90 iPrOH/Hexane
Column Type: OD-H 2
Method Developer: Administrator
Pump A: L-2130
Pump A Solvent A: Hexane
Pump A Solvent B: 10/90 iPrOH/Hexane
Pump A Solvent C: iPrOH
Pump A Solvent D: iPrOH
Method Description:

Chrom Type: HPLC Channel : 1
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %
1	19.55	699405	50.279
2	24.56	691632	49.721
		1391037	100.000

Peak rejection level: 0