Layered Lanthanum Nickelates Reimagined: La_2NiO_4 as a Cooperative Acid–Base Catalyst for Efficient C–C Bond Formation in Water

Taku Kitanosono, Sota Iwasaki, Rina Osada, Yasuhiro Yamashita, Shū Kobayashi**

Department of Chemistry, School of Sciences, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo, Japan

Supporting Information

Table of Contents

1. General experimental

Nuclear magnetic resonance (NMR) spectra were recorded on a JEOL ECZ-500R or ECZ-400R spectrometer. Tetramethylsilane (TMS) served as the internal standard ($\delta = 0$) for ^{1}H NMR, $CDCl_3$ ($\delta = 77.0$) was used as the internal standard for ^{13}C NMR, and benzotrifluoride ($\delta = -63.72$) was used as the internal standard for ^{19}F NMR. Infrared (IR) spectra were obtained using a SHIMADZU IRSpirit spectrometer. Data are represented as frequency of absorption (cm^{-1}). X-ray diffraction (XRD) was recorded using MiniFlex 300/600 spectrometer in the Bragg angle range of 3-60°. High Resolution Mass Spectra (HRMS) were recorded using a JEOL JMS-T100TD (DART) spectrometer. Melting points were obtained using YAZAWA micro melting point BY-1 apparatus. STEM/EDS or TEM images were obtained using a JEOL JEM-2100F instrument. Ammonia-probed temperature-programed desorption measurement was conducted on a BELCAT-II of MicrotracBEL. Prior to NH_3-TPD measurements, La_2NiO_4 (46.4 mg) was pretreated at 500 °C for 1 h under a flow of helium. The sample was then cooled to 100 °C and exposed to a 5% NH_3/He gas mixture for 30 min. Subsequently, the temperature was increased at a heating rate of 10 °C min^{-1} under a helium atmosphere, and the NH_3-TPD spectrum was recorded. Centrifugation was performed using a KOKUSAN H-36 centrifuge. Preparative thin-layer chromatography (PTLC) was carried out using Wakogel B-5F from Wako Pure Chemical Industries, Ltd. Deionized water from a MILLIPORE MilliQ machine (Gradient A 10) was used as solvent without further treatment. All organic solvents used were commercially available dry solvents, which were distilled appropriately under an argon atmosphere or were stored over molecular sieves prior to use. All reagents used as additives were either distilled or recrystallized before use.

2. Catalyst Preparation

Preparation of La_2NiO_4, $La_3Ni_2O_7$, $La_4Ni_3O_{10}$[1]

In a 50 mL round-bottom flask, $La(NO_3)_3 \cdot 6H_2O$ (3.00 g, 6.93 mmol) and $Ni(NO_3)_2 \cdot 6H_2O$ (0.50, 0.67, and 0.75 equiv, respectively) were dissolved in 10 mL of deionized water. Citric acid (2.99 g, 15.6 mmol) and ethylenediaminetetraacetic acid (EDTA; 3.00 g, 10.4 mmol) were then added, followed by the dropwise addition of 28% aqueous ammonia until the pH reached 7, under continuous stirring. The resulting solution was heated at 100 °C to evaporate water, yielding a gel that was transferred to a crucible and dried overnight in a muffle furnace at 100 °C. Upon further heating at 350 °C for 6 hours, the foam-like gel underwent self-ignition. The resulting solid was finely ground and subsequently calcined at 1100 °C (2 °C/min ramp rate) for 9 hours (La_2NiO_4) and for 30 hours ($La_3Ni_2O_7$ and $La_4Ni_3O_{10}$).

ICP result
La_2NiO_4: La 0.0049 mol/g, Ni 0.0023 mol/g
$La_3Ni_2O_7$: La 0.0047 mol/g, Ni 0.0029 mol/g
$La_4Ni_3O_{10}$: La 0.0046 mol/g, Ni 0.0032 mol/g

Preparation of $LaNiO_3$[2]

In a 100 mL round-bottom flask, $La(NO_3)_3 \cdot 6H_2O$ (2.17 g, 5.0 mmol) and $Ni(NO_3)_2 \cdot 6H_2O$ (1.45 g, 5.0 mmol) were dissolved in 50 mL of deionized water and allowed to be stirred for 1 hour. Citric acid (5.76 g, 30 mmol) and ethylene glycol (1.86 g, 30 mmol) were then added, followed by further stirring for 3 hours at 90 °C. The resulting solution was heated at 100 °C to evaporate water, yielding a gel that was transferred to a crucible and dried overnight in a muffle furnace at 110 °C for 24 hours. The resulting foam-like gel was finely ground and subsequently calcined at 400 °C (2 °C/min ramp rate) for 2 hours, followed by calcination at 800 °C for another 5 hours.

ICP result
$LaNiO_3$: La 0.0038 mol/g, Ni 0.0036 mol/g

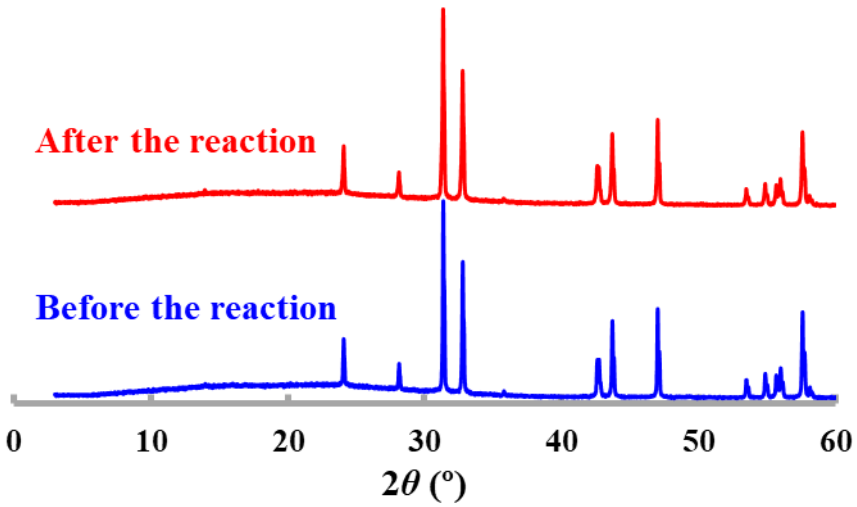


Figure S1. XRD patterns of La_2NiO_4 before and after the reaction.

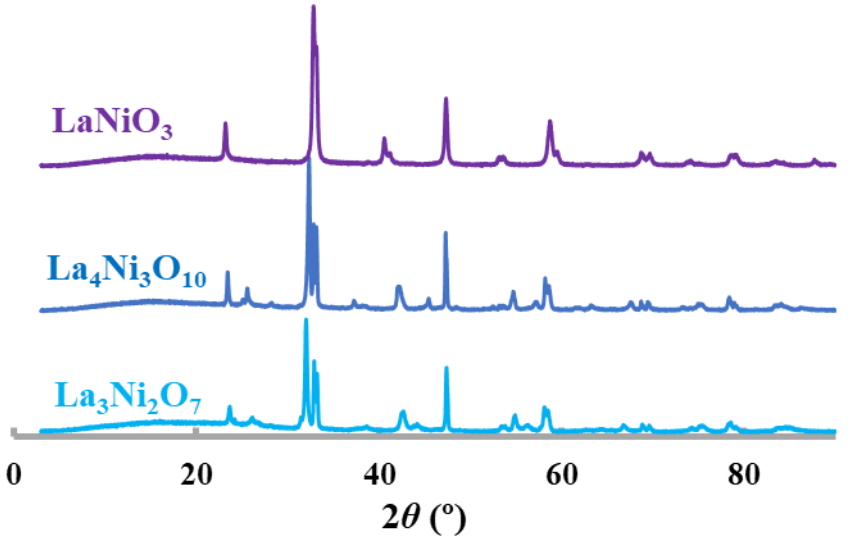


Figure S2. XRD patterns of $La_3Ni_2O_7$, $La_4Ni_3O_{10}$ and $LaNiO_3$.

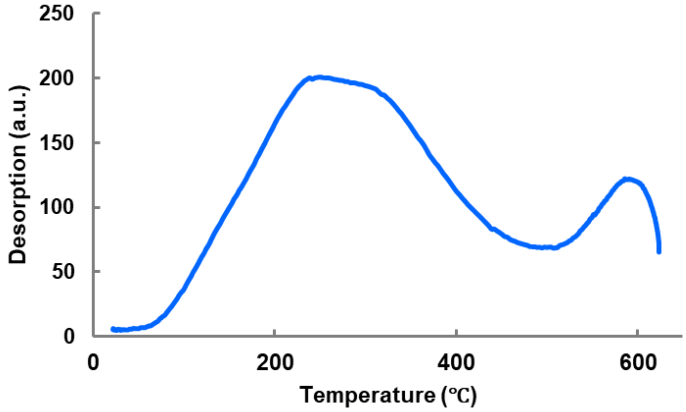
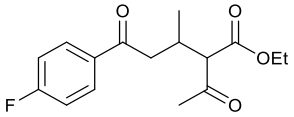


Figure S3. NH_3-TPD profile

3. Typical procedure for carbon-carbon bond formation

In a 2 mL vial equipped with a magnetic stirring bar, La_2NiO_4 (La: 0.012 mmol), previously stored under anaerobic conditions, was introduced under an inert atmosphere inside a glove box. Subsequently, (*E*)-1-(4-fluorophenyl)but-2-en-1-one (118.2 mg, 0.72 mmol), ethyl acetoacetate (78.1 mg, 0.60 mmol), and degassed deionized water (1.0 mL) were added. The vial was purged with argon and the reaction mixture was stirred vigorously in a water bath maintained at 40 °C. After 1 hour, the reaction was quenched by the addition of 1 M aqueous HCl (1.0 mL). The product was extracted with dichloromethane (3 × 10 mL), and the combined organic layers were dried over anhydrous sodium sulfate. Following filtration, the filtrate was concentrated under reduced pressure. The crude product was analyzed by ^{1}H NMR using dibromomethane as an internal standard. The residue was purified by preparative thin-layer chromatography (^{n}hexane/EtOAc = 4:1), affording the desired compound.

Ethyl 2-acetyl-5-(4'-fluorophenyl)-3-methyl-5-oxopentanoate[3]
(mixture of diastereomers)



Colorless oil

^{1}H NMR (399 MHz, $CDCl_3$): δ = 8.02 (q, *J* = 7.2 Hz, 2H), 7.14 (t, *J* = 8.5 Hz, 2H), 4.21+4.21 (q, *J* = 7.2 Hz, 7.0 Hz, 2H), 3.60+3.54 (d, *J* = 7.5 Hz, 7.5 Hz, 1H), 3.21+3.16 (dd, *J* = 16.4, 3.8 Hz, 16.5, 5.3 Hz, 1H), 3.02-2.92 (m, 1H), 2.84+2.81 (dd, *J* = 16.5, 7.5 Hz, 16.4, 8.8 Hz, 1H), 2.27 (s, 3H), 1.28+1.27 (t, *J* = 7.1 Hz, 7.2 Hz, 3H), 1.05+1.03 (d, *J* = 6.9 Hz, 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 202.7, 197.1, 197.1, 168.9, 168.8, 165.6 (d, $J_{C\text{-}F}$ = 254.8 Hz), 165.5(d, $J_{C\text{-}F}$ = 254.8 Hz), 133.2 (d, $J_{C\text{-}F}$ = 3.4 Hz), 133.1 (d, $J_{C\text{-}F}$ = 2.9 Hz), 130.7 (d, $J_{C\text{-}F}$ = 9.6 Hz), 130.6 (d, $J_{C\text{-}F}$ = 9.2 Hz), 115.5 (d, $J_{C\text{-}F}$ = 21.7 Hz), 115.5 (d, $J_{C\text{-}F}$ = 21.7 Hz), 64.2, 63.8, 61.2, 61.1, 42.6, 42.3, 29.5, 29.5, 29.2, 28.9, 17.8, 17.3, 13.9.

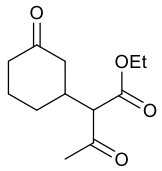
^{19}F NMR (376 MHz, $CDCl_3$): δ = –106.2, –106.3.

Modified procedure for low-reactive substrates

In a 2 mL vial equipped with a magnetic stirring bar, La_2NiO_4 (La: 0.030 mmol), previously stored under anaerobic conditions, was introduced inside a glove box. Subsequently, 1,10-phenanthroline monohydrate (7.14 mg, 0.036 mmol), (*E*)-1-(4-fluorophenyl)but-2-en-1-one (118.2 mg, 0.72 mmol), diethyl malonate (96.1 mg, 0.60

mmol), and degassed ultrapure water (1.0 mL) were added. The vial was then purged with argon, and the reaction mixture was stirred vigorously in a water bath maintained at 40 °C. After 4 hours, the reaction was quenched by the addition of 1 M aqueous HCl (1.0 mL). The product was extracted with dichloromethane (3 × 10 mL), and the combined organic layers were dried over anhydrous sodium sulfate. Following filtration, the filtrate was concentrated under reduced pressure. The crude product was analyzed by ^{1}H NMR using dibromomethane as an internal standard. The residue was purified by preparative thin-layer chromatography (^{n}hexane/EtOAc = 4:1), affording the desired compound.

Ethyl 3-oxo-2-(3-oxocyclohexyl)butanoate[4]
(mixture of diastereomers)



Colorless oil

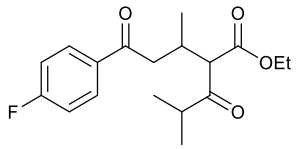
^{1}H NMR (399 MHz, $CDCl_3$): δ = 4.22+4.20 (q, J = 7.1 Hz, 7.1 Hz, 2H), 3.41 (t, J = 8.1 Hz, 1H), 2.64-2.54 (m, 1H), 2.42-2.34 (m, 2H), 2.29 (dd, J = 12.1, 6.4 Hz, 1H), 2.25+2.23 (s, 3H), 2.19-2.12 (m, 1H), 2.08-2.05 (m, 1H), 1.93-1.85 (m, 1H), 1.76-1.63 (m, 1H), 1.53-1.38 (m, 1H), 1.29+1.29+1.28+1.28 (t, J = 7.1 Hz, 7.1 Hz, 7.2 Hz, 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 209.4, 209.3, 201.5, 201.4, 168.1, 167.9, 64.9, 64.5, 61.5, 61.4, 45.2, 44.8, 40.9, 40.8, 37.5, 29.4, 28.8, 28.3, 24.4, 24.4, 13.9, 13.9.

4. Analytical data

When the product is a diastereomeric mixture, two diastereomers cannot be distinguished further in NMR spectra and some of the peaks overlap.

Ethyl 5-(4'-fluorophenyl)-2-isobutyryl-3-methyl-5-oxopentanoate (mixture of diastereomers)



Colorless oil

IR (dichloromethane solution) ν = 2970, 2162, 1736, 1713, 1600 cm^{-1}.

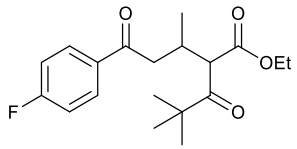
^1H NMR (399 MHz, $CDCl_3$): δ = 8.05-8.01 (m, 2H), 7.16-7.11 (m, 2H), 4.22-4.15 (m, 2H), 3.82+3.80 (d, J = 7.3 Hz, 7.5 Hz, 1H), 3.25+3.19 (dd, J = 16.0, 3.7 Hz, 16.0, 4.8 Hz, 1H) 2.96-2.92 (m, 1H), 2.85-2.73 (m, 1H), 2.84-2.76 (m, 1H), 1.26+1.25 (t, J = 7.1 Hz, 7.1 Hz, 3H), 1.15-1.08 (m, 6H), 1.04+1.02 (d, J = 6.9 Hz, 6.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 208.9, 208.8, 197.5, 197.5, 168.9, 168.7, 165.7 (d, J_{C-F} = 254.8 Hz), 165.7(d, J_{C-F} = 254.3 Hz), 133.2 (d, J_{C-F} = 2.9 Hz), 133.2 (d, J_{C-F} = 2.9 Hz), 130.8(d, J_{C-F} = 9.2 Hz), 115.6 (d, J_{C-F} = 22.2 Hz), 115.6 (d, J_{C-F} = 22.2 Hz), 61.4, 61.3, 61.2, 43.0, 42.4, 41.3, 41.1, 29.6, 29.3, 18.3, 18.2, 18.0, 18.0, 17.9, 17.3, 14.0.

^{19}F NMR (376 MHz, $CDCl_3$): δ = –106.2, –106.3.

HRMS (DART) calcd for $C_{18}H_{23}FO_4$ $[M+H]^+$: 323.1659; found 323.1665.

Ethyl 2-(3-(4'-fluorophenyl)-3-oxopropyl)-4,4-dimethyl-3-oxopentanoate[3] **(mixture of diastereomers)**



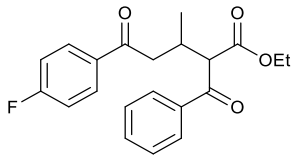
Colorless oil

^1H NMR (399 MHz, $CDCl_3$): δ = 8.05-7.99 (m, 2H), 7.17-7.11 (m, 2H), 4.20-4.13 (m, 2H), 4.07-4.02 (m, 1H), 3.31+3.16 (dd, J = 16.2, 3.2 Hz, 15.9, 4.2 Hz), 2.97-2.93 (m, 1H), 2.85+2.84+2.73+2.72 (dd, J = 16.4, 8.8 Hz, 16.4, 8.4 Hz, 15.8, 8.5 Hz, 15.8, 8.5 Hz), 1.28-1.22 (m, 3H), 1.20+1.19+1.18+1.18 (s, 9H), 1.07-0.99 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 209.7, 209.4, 197.4, 197.3, 168.8, 168.6, 166.8, 165.6

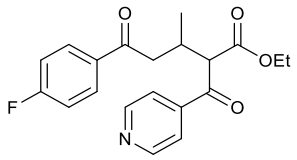
(d, $J_{C\text{-}F}$ = 254.8 Hz), 165.5 (d, $J_{C\text{-}F}$ = 254.3 Hz), 133.3 (d, $J_{C\text{-}F}$ = 2.9 Hz), 133.1 ($J_{C\text{-}F}$ = 2.9 Hz), 130.8 ($J_{C\text{-}F}$ = 9.2 Hz), 130.6 ($J_{C\text{-}F}$ = 9.6 Hz), 115.5 ($J_{C\text{-}F}$ = 21.7), $J_{C\text{-}F}$ = ($J_{C\text{-}F}$ =22.2), 61.2, 61.1, 57.4, 57.1, 45.5, 43.3. 42.0, 30.6, 30.5, 26.0, 26.0, 18.6, 17.0, 13.9.
^{19}F NMR (376 MHz, $CDCl_3$): δ = −106.3, −106.5.

Ethyl 2-benzoyl-5-(4'-fluorophenyl)-3-methyl-5-oxopentanoate[3]
(mixture of diastereomers)



Colorless oil
^{1}H NMR (399 MHz, $CDCl_3$): δ = 8.09-7.99 (m, 4H), 7.62-7.57 (m, 1H), 7.51-7.46 (m, 2H), 7.16-7.09 (m, 2H), 4.55+4.52 (J = 7.3 Hz, 7.3 Hz, 1H)), 4.19-4.09 (m, 2H), 3.33 (dd, J = 16.2, 3.7 Hz, 16.5, 5.3 Hz, 1H), 3.16-3.09 (m, 1H), 2.92+2.81 (dd, J = 16.2, 9.1 Hz, 16.2, 8.0 Hz, 1H), 1.17+1.15 (t, J = 7.2 Hz, 7.2 Hz, 3H), 1.12+1.08(d, J = 6.9 Hz, 6.9 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.6, 197.5, 194.9, 194.8, 169.1, 168.9, 165.7 ($J_{C\text{-}F}$ = 254.8 Hz), 165.6 ($J_{C\text{-}F}$ = 254.8 Hz), 136.6, 136.4, 133.6, 133.6, 133.3 ($J_{C\text{-}F}$ = 2.9 Hz), 133.2 ($J_{C\text{-}F}$ = 2.9 Hz), 130.8 ($J_{C\text{-}F}$ = 9.2 Hz), 130.8 ($J_{C\text{-}F}$ = 9.2 Hz), 128.7, 128.6, 128.5, 115.6 ($J_{C\text{-}F}$ = 22.2 Hz), 115.6 ($J_{C\text{-}F}$ = 21.7 Hz), 61.3, 61.2, 58.4, 58.3, 43.1, 42.4, 30.2, 29.8, 18.2, 17.1, 13.9, 13.9.
^{19}F NMR (376 MHz, $CDCl_3$): δ = −106.2, −106.3.

Ethyl 5-(4'-fluorophenyl)-2-isonicotinoyl-3-methyl-5-oxopentanoate
(mixture of diastereomers)



Colorless oil
IR (methanol solution) ν = 2941, 1733, 1684, 1225 cm^{-1}.
^{1}H NMR (399 MHz, $CDCl_3$): δ = 8.84 (td, J = 4.3, 1.5 Hz, 2H), 8.04-8.01 (m, 2H), 7.85-7.76 (m, 2H), 7.14 (td, J = 8.6, 2.4 Hz, 2H), 4.57+4.50 (d, J = 6.4 Hz, 7.3 Hz, 1H), 4.19-4.11 (m, 2H), 3.34+3.33 (dd, J = 16.9, 6.4 Hz, 16.6, 4.2 Hz, 1H), 3.16-3.07 (m, 1H), 2.95+2.92 (dd, J = 16.6, 8.2 Hz, 16.9, 6.9 Hz, 1H), 1.17+1.15 (t, J = 7.4 Hz, 7.4 Hz, 3H),

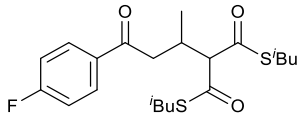
1.14+1.11 (d, J = 6.8 Hz, 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.4, 197.1, 194.6, 194.6, 168.4, 168.3, 165.8 (d, $J_{C\text{-}F}$ = 255.3 Hz), 165.7(d, $J_{C\text{-}F}$ = 254.8 Hz), 151.0, 142.5, 142.2, 133.2 (d, $J_{C\text{-}F}$ = 1.4 Hz), 133.2 (d, $J_{C\text{-}F}$ = 1.4 Hz), 130.7 (d, $J_{C\text{-}F}$ = 9.2 Hz), 121.2, 121.1, 115.7 (d, $J_{C\text{-}F}$ = 22.2 Hz), 115.7 (d, $J_{C\text{-}F}$ = 21.6 Hz), 61.7, 61.5, 58.3, 58.0, 42.7, 42.1, 29.8, 29.2, 18.2, 17.1, 13.9, 13.9.

^{19}F NMR (376 MHz, $CDCl_3$): δ = –105.9, –106.1.

HRMS (DART) calcd for $C_{20}H_{21}FNO_4$ $[M+H]^+$: 358.1455; found 358.1451.

_S_,_S_-Diisobutyl 2-(4-(4'-fluorophenyl)-4-oxobutan-2-yl)propanebis(thioate)



Colorless oil

IR (dichloromethane solution) ν = 2926, 1682, 1597, 983 cm^{-1}.

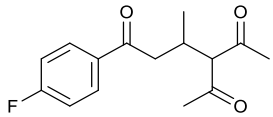
^{1}H NMR (399 MHz, $CDCl_3$): δ = 8.00-7.97 (m, 2H), 7.15-7.11 (m, 2H), 3.96 (d, J = 8.9 Hz, 1H), 3.18 (dd, J = 16.0, 3.4 Hz, 1H), 3.09-3.05 (m, 1H), 2.91-2.80 (m, 4H), 2.76 (dd, J = 16.1, 9.3 Hz, 1H), 1.88-1.76 (m, 2H), 1.04 (d, J = 6.6 Hz, 3H), 0.95 (s, 6H), 0.94 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ = 196.8, 193.5, 193.1, 165.7 (d, $J_{C\text{-}F}$ = 255.0 Hz), 133.2 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.8 (d, $J_{C\text{-}F}$ = 9.4 Hz), 115.6. (d, J = 22.0 Hz), 73.4, 42.3, 37.7, 37.7, 31.7, 28.5, 28.5, 21.6, 21.6, 17.5.

^{19}F NMR (376 MHz, $CDCl_3$): δ = –106.1.

HRMS (DART) calcd for $C_{21}H_{30}FO_3S_2$ $[M+H]^+$:413.16204; found 413.16271.

4-Acetyl-1-(4'-fluorophenyl)-3-methylhexane-1,5-dione



Colorless oil

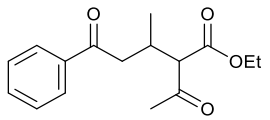
IR (dichloromethane solution) ν = 2921, 1697, 1507, 1358, 834 cm^{-1}.

^{1}H NMR (399 MHz, $CDCl_3$): δ = 8.01-7.98 (m, 2H), 7.16-7.12 (m, 2H), 3.83 (d, J = 8.5 Hz, 1H), 3.02 (m, 2H), 2.81 (m, 1H), 2.24 (s, 3H), 2.21 (s, 3H), 1.00 (d, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 204.3, 203.9, 197.0, 165.7 (d, $J_{C\text{-}F}$ = 255.3 Hz), 133.1 (d, $J_{C\text{-}F}$ = 2.9 Hz), 130.7 (d, $J_{C\text{-}F}$ = 9.6 Hz), 115.6 (d, $J_{C\text{-}F}$ = 21.7 Hz), 73.4, 42.4, 30.2, 29.7, 29.6, 17.7.

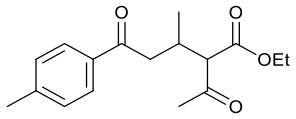
^{19}F NMR (376 MHz, $CDCl_3$): δ = –106.0.
HRMS (DART) calcd for $C_{15}H_{18}FO_3$ $[M+H]^+$: 265.1240; found 265.1241.

Ethyl 2-acetyl-3-methyl-5-oxo-5-phenylpentanoate[3]
(mixture of diastereomers)



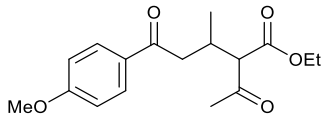
Colorless oil
^{1}H NMR (399 MHz, $CDCl_3$): δ = 7.99-7.95 (m, 2H), 7.58-7.54 (m, 1H), 7.48-7.44 (m, 2H), 4.21+4.20+4.20+4.20 (q, J = 7.1 Hz, 7,1 Hz, 7.1 Hz, 7.1 Hz, 2H), 3.63+3.56 (d, J = 7.3 Hz, 7.5 Hz, 1H), 3.22+3.17 (dd, J = 16.4, 3.3 Hz, 16.5, 5.0 Hz, 1H), 3.03-2.96 (m, 1H), 2.93-2.84 (m, 1H), 2.27+2.26 (s, 3H), 1.27+1.26 (t, J = 7.1 Hz, 7.1 Hz, 3H), 1.06+1.04 (d, J = 6.6 Hz, 6.6 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ = 202.8, 202.8, 198.8, 198.7, 168.9, 168.8, 136.8, 136.7, 133.0, 133.0, 128.5, 128.0, 127.9, 64.3, 63.9, 61.2, 61.1, 42.6, 42.4, 29.5, 29.5, 29.2, 28.9, 17.9, 17.3, 13.9.

Ethyl 2-acetyl-3-methyl-5-oxo-5-(*p*-tolyl)pentanoate
(mixture of diastereomers)



Colorless oil
IR (dichloromethane solution) ν = 2965, 1731, 1674, 1357, 1151, 805 cm^{-1}.
^{1}H NMR (399 MHz, $CDCl_3$): δ = 7.87 (t, J = 7.8 Hz, 2H), 7.30-7.25 (m, 2H), 4.20+4.20+4.20+4.20 (q, J = 7.2 Hz, 7.1 Hz, 7.1 Hz, 7.1 Hz, 2H), 3.62+3.55 (d, J = 7.3, 7.8 Hz, 1H), 3.20-3.11 (m, 1H), 2.99-2.96 (m, 1H), 2.86+2.83 (dd, J = 16.1, 9.0 Hz, 16.4, 7.7 Hz, 1H), 2.40 (s, 3H), 2.26+2.26 (s, 3H), 1.27+1.26 (t, J = 7.2 Hz, 7.2 Hz, 3H), 1.05+1.02 (d, J = 6.6 Hz, 6.6 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ = 202.9, 198.5, 198.4, 169.0, 168.9, 143.8, 143.8, 134.4, 134.3, 129.2, 128.2, 128.1, 64.5, 64.0, 61.2, 61.1, 42.5, 42.3, 29.5, 29.5, 29.4, 29.0, 21.5, 17.9, 17.4, 14.0.
HRMS (DART) calcd for $C_{17}H_{23}O_4$ $[M+H]^+$: 291.15963; found 291.15960.

Ethyl 2-acetyl-5-(4'-methoxyphenyl)-3-methyl-5-oxopentanoate[3]
(mixture of diastereomers)

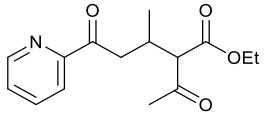


Colorless oil

^{1}H NMR (399 MHz, $CDCl_3$): δ = 7.99-7.94 (m, 2H), 6.95-6.92 (m, 2H), 4.21+4.20 (q, J = 7.1 Hz, 7.2 Hz, 2H), 3.87 (s, 3H), 3.62+3.55 (d, J = 7.5 Hz, 7.8 Hz, 1H), 3.16+3.11 (dd, J = 16.0, 3.7 Hz, 16.4, 5.4 Hz, 1H), 3.02-2.92 (m, 1H), 2.81+2.79 (dd, J = 16.1, 8.8 Hz, 16.2, 7.5 Hz, 1H), 2.27+2.26 (s, 3H), 1.27+1.26 (t, J = 7.1 Hz, 3H), 1.05+1.02 (d, J = 6.9 Hz, 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 202.9, 202.9, 197.3, 197.3, 169.0, 168.9, 163.4, 163.4, 130.3, 130.3, 129.9, 129.8, 113.6, 64.5, 64.0, 61.2, 61.1, 55.3, 42.3, 42.1, 29.5, 29.5, 29.1, 17.9, 17.3, 14.0.

Ethyl 2-acetyl-3-methyl-5-oxo-5-(pyridin-2-yl)pentanoate
(mixture of diastereomers)



Pale yellow oil

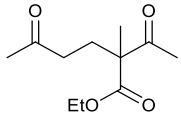
IR (dichloromethane solution) ν = 2933, 1740, 1690, 1362, 1154 cm^{-1}.

^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.67 (d, J = 4.0 Hz, 1H), 8.03 (d, J = 7.7 Hz, 1H), 7.84 (t, J = 7.7 Hz, 1H), 7.49 (m, 1H), 4.20 (m, 2H), 3.60+3.55 (d, J = 8.0 Hz, 8.6 Hz, 1H), 3.34-3.30 (m, 1.4H), 3.19 (dd, J =17.4, 7.5 Hz, 0.6H), 3.08-2.98 (m, 1H), 2.28 (s, 3H), 1.27+1.25 (t, J = 7.2 Hz, 7.4 Hz, 3H), 1.06+1.04 (d, J = 7.0 Hz, 7.2 Hz).

^{13}C NMR (126 MHz, $CDCl_3$): δ = 203.1, 202.9, 169.0, 169.0, 153.3, 153.2, 148.8, 136.8, 136.8, 127.1, 127.1, 121.7, 121.6, 64.8, 64.6, 61.2, 61.2, 41.9, 41.7, 29.4, 29.2, 29.0, 28.8, 18.1, 17.5, 14.0, 14.0.

HRMS (DART) calcd for $C_{15}H_{20}NO_4$ $[M+H]^+$: 278.13923 ; found 278.13936.

Ethyl 2-acetyl-2-methyl-5-oxohexanoate[5]



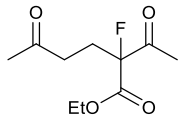
Colorless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.20 (q, J= 7.1 Hz, 2H), 2.45-2.40 (m, 2H), 2.16 (s, 3H), 2.15 (s, 3H), 2.16-2.00 (m, 2H), 1.34 (s, 3H), 1.28 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 202.2, 205.2, 172.4, 61.2, 58.4, 38.4, 29.7, 28.2, 26.0,

19.1, 13.8.

Ethyl 2-acetyl-2-fluoro-5-oxohexanoate[6]



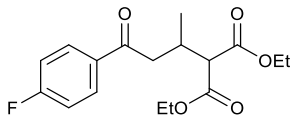
Colorless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.28 (q, J = 7.1 Hz, 2H), 2.55 (t, J = 7.5 Hz, 2H), 2.47-2.34 (m, 2H), 2,31 (d, $J_{C\text{-}F}$ = 4.4 Hz), 2.16 (s, 3H), 1.31 (t, J = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ = 206.1, 201.2 (d, $J_{C\text{-}F}$ = 28.1 Hz), 165.9 (d, $J_{C\text{-}F}$ = 25.7 Hz), 99.0 (d, $J_{C\text{-}F}$ = 197.1 Hz), 62.7, 36.5 (d, $J_{C\text{-}F}$ = 3.3 Hz), 29.7, 27.2 (d, $J_{C\text{-}F}$ = 21.1 Hz), 25.4, 13.9.

^{19}F NMR (471 MHz, $CDCl_3$): δ = −167.6.

Ethyl 2-acetyl-5-(4'-fluorophenyl)-3-methyl-5-oxopentanoate[3]



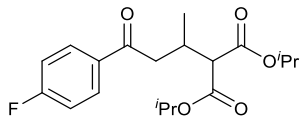
Colorless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.05-8.02 (m, 2H), 7.14 (t, J = 8.6 Hz, 2H), 4.25-4.19 (m, 4H), 3.48 (d, J = 6.6 Hz, 1H), 3.29 (dd, J = 16.2, 4.2 Hz, 1H), 2.99-2.93 (m, 1H), 2.88 (dd, J = 16.3, 8.7 Hz, 1H), 1.30-1.25 (m, 6H), 1.10 (d, J = 6.7 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ = 197.0, 168.5, 168.4, 165.6 (d, $J_{C\text{-}F}$ = 254.7 Hz), 133.2 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.7 (d, $J_{C\text{-}F}$ = 9.4 Hz), 115.5 (d, $J_{C\text{-}F}$ = 21.7 Hz), 61.2, 56.3, 42.5, 29.4, 17.6, 13.9, 13.9.

^{19}F NMR (471 MHz, $CDCl_3$): δ = –106.3.

Diisopropyl 2-(4-(4'-fluorophenyl)-4-oxobutan-2-yl)malonate



Colorless oil

IR (dichloromethane solution) ν = 2982, 1720, 1682, 1100 cm^{-1}.

^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.06-8.04 (m, 2H), 7.16-7.12 (m, 2H), 5.10+5.08 (sep, J = 6.3 Hz, 6.3 Hz, 2H), 3.41 (d, J = 6.6 Hz, 1H), 3.31 (dd, J = 16.0, 3.9 Hz, 1H), 2.96-2.92 (m, 1H), 2.87 (dd, J = 16.0, 8.9 Hz, 1H), 1.28-1.24 (m, 12H), 1.10 (d, J = 6.7 Hz,

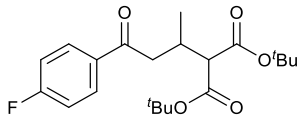
3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ = 197.3, 168.2, 168.1, 165.7 (d, $J_{C\text{-}F}$ = 254.7 Hz), 133.4 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.8 (d, $J_{C\text{-}F}$ = 9.4 Hz), 115.7 (d, $J_{C\text{-}F}$ = 21.7 Hz), 68.9, 56.8, 42.7, 29.4, 21.7, 21.6, 21.6, 17.6.

^{19}F NMR (376 MHz, $CDCl_3$): δ = –106.3.

HRMS (DART) calcd for $C_{19}H_{26}FO_5$ $[M+H]^+$: 353.17643; found 353.17454.

Di-tert-butyl 2-(4-(4'-fluorophenyl)-4-oxobutan-2-yl)malonate



White solid: m.p. 84-85 °C

IR (dichloromethane solution) ν = 2936, 1718, 1684, 1600, 1135, 805 cm^{-1}.

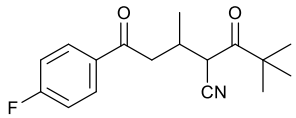
^{1}H NMR (399 MHz, $CDCl_3$): δ = 8.06-8.03 (m, 2H), 7.13 (t, J = 8.6 Hz, 2H), 3.29 (dd, J = 15.0, 2.6 Hz, 1H), 3.25 (d, J = 6.6 Hz, 1H), 2.92-2.85 (m, 1H), 2.86-2.79 (m, 1H), 1.49+1.47 (s, 18H), 1.07 (d, J =6.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.3, 167.9, 167.9, 165.6 (d, $J_{C\text{-}F}$ = 254.3 Hz), 133.3 (d, $J_{C\text{-}F}$ = 2.9), 130.7 (d, $J_{C\text{-}F}$ = 9.6), 115.5 (d, $J_{C\text{-}F}$ = 21.7), 81.5, 81.5, 58.4, 42.8, 29.3, 27.8, 27.8, 17.5.

^{19}F NMR (376 MHz, $CDCl_3$): δ = –106.5.

HRMS (DART) calcd for $C_{21}H_{30}FO_5$ $[M+H]^+$: 381.20773; found 381.20908.

5-(4'-Fluorophenyl)-3-methyl-5-oxo-2-pivaloylpentanenitrile (mixture of diastereomers)



White Solid: m.p. 59-61 °C.

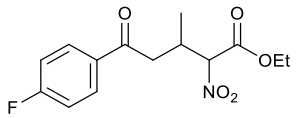
IR (dichloromethane solution) ν = 2928, 2244, 1684, 1600, 837 cm^{-1}.

^{1}H NMR (399 MHz, $CDCl_3$): δ = 8.03-7.98 (m, 2H), 7.18-7.12 (m, 2H), 4.35 (d, J = 4.6 Hz, 0.6H), 4.11 (d, J = 5.9 Hz, 0.4H), 3.43 (dd, J = 17.5, 3.8 Hz, 0.4H), 3.19 (dd, J = 18.1, 8.2 Hz, 0.6H), 3.05-2.98 (m, 1H), 2.95-2.83 (m, 1H), 1.30+1.26 (s, 9H), 1.20+1.16 (d, J = 6.9 Hz, 6.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.6, 205.5, 196.5, 196.2, 165.9 (d, $J_{C\text{-}F}$ = 255.8 Hz), 165.7 (d, $J_{C\text{-}F}$ = 255.3 Hz), 133.1 (d, $J_{C\text{-}F}$ = 2.9 Hz), 132.7 (d, $J_{C\text{-}F}$ = 2.9 Hz), 130.6 (d, $J_{C\text{-}F}$ = 1.4 Hz), 130.6 (d, $J_{C\text{-}F}$ = 1.4 Hz), 116.4, 116.2, 115.8 (d, $J_{C\text{-}F}$ = 22.2 Hz), 115.7 (d, $J_{C\text{-}$

$_F$ = 21.7 Hz), 45.6, 45.5, 42.8, 42.5, 42.4, 41.1, 29.8, 29.3, 26.2, 25.9, 19.0, 16.5.
^{19}F NMR (376 MHz, $CDCl_3$): δ = –105.2, −105.8
HRMS (DART) calcd for $C_{17}H_{21}FNO_2$ $[M+H]^+$: 290.15563; found 290.15478.

Ethyl 5-(4'-fluorophenyl)-3-methyl-2-nitro-5-oxopentanoate[3]
(mixture of diastereomers)



Colorless oil
^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.01-7.98 (m, 2H), 7.16-7.12 (m 2H), 5.39+5.33 (d, J = 5.6 Hz, 5.4 Hz, 1H), 4.32-4.27 (m, 2H), 3.29-3.23 (m, 2H), 3.11-3.03 (m, 1H), 1.30+1.30 (t, J = 7.2 Hz, 7.2 Hz, 3H), 1.20+1.19 (d, J = 7.0 Hz, 7.2 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ = 195.8, 195.7, 165.9 (d, $J_{C\text{-}F}$ = 255.6 Hz), 165.9 (d, $J_{C\text{-}F}$ = 255.6 Hz), 163.7, 132.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 132.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.6 (d, $J_{C\text{-}F}$ = 9.4 Hz), 130.6 (d, $J_{C\text{-}F}$ = 9.4 Hz), 115.8 (d, $J_{C\text{-}F}$ = 22.0 Hz), 115.8 (d, $J_{C\text{-}F}$ = 22.0 Hz), 91.1, 90.8, 62.9, 62.9, 40.7, 40.6, 30.5, 30.5, 16.3, 16.1, 13.8, 13.8.
^{19}F NMR (376 MHz, $CDCl_3$): δ = –105.5, –105.6.

5. Gram-scale experiment

In a 6 mL vial equipped with a magnetic stirring bar, La_2NiO_4 (La: 0.1 mmol), previously stored under anaerobic conditions, was introduced under an inert atmosphere inside a glove box. Subsequently, (*E*)-1-(4-fluorophenyl)but-2-en-1-one (984.7 mg, 6.0 mmol), ethyl acetoacetate (650.8 mg, 5.0 mmol), and degassed deionized water (4.0 mL) were added. The vial was purged with argon and the reaction mixture was stirred vigorously in a water bath maintained at 40 °C. After 1 hour, the mixture was centrifuged at 3,500 rpm for 5 minutes, resulting in separation into a solid phase, an organic layer (lower), and an aqueous layer (upper). The upper aqueous layer was carefully removed using a pipette. Ethanol (4.0 mL) was then added to the remaining mixture, followed by centrifugation at 3,500 rpm for 5 minutes. The supernatant was collected, taking care not to disturb the solid catalyst. This ethanol washing step was repeated three times. Subsequently, ^{n}hexane was added to wash the catalyst, and the mixture was centrifuged again at 3,500 rpm for 5 minutes. The resulting supernatant was collected, and the remaining solid catalyst was dried under vacuum. All ethanol and ^{n}hexane extracts were combined and dried over anhydrous sodium sulfate. After filtration, the filtrate was concentrated under reduced pressure. The crude product was purified by column chromatography (^{n}hexane/EtOAc = 4:1), affording the desired compound (1.4010 g, 95%). The XRD pattern of the catalyst after the reaction is shown in Figure S1.

Figure S4. Appearance of the reaction. The starting material is immiscible with water.

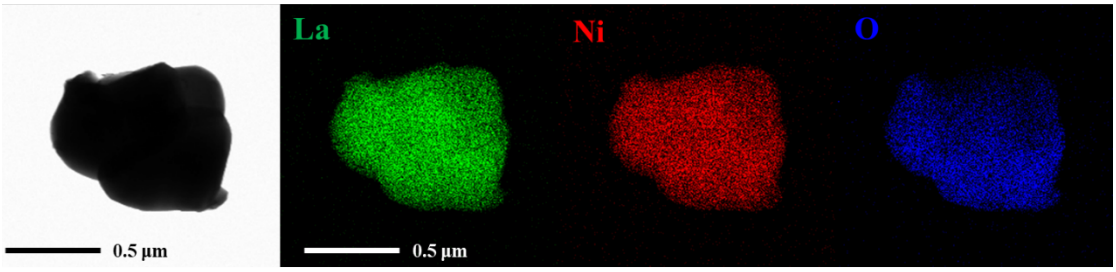


Figure S5. STEM image of the catalyst before the reaction.

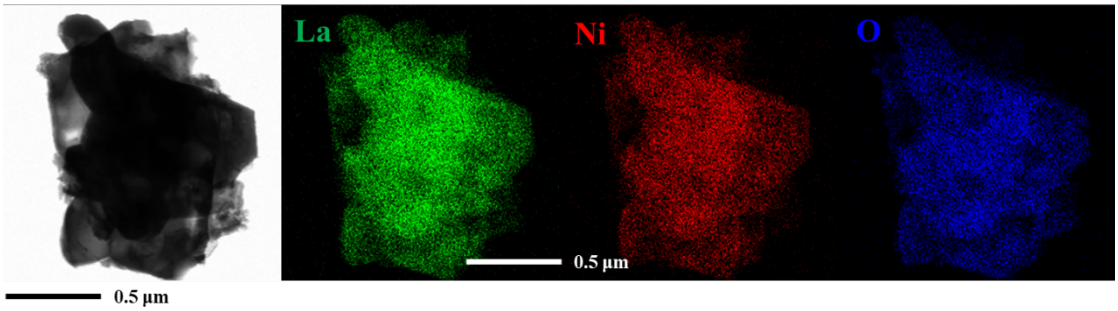


Figure S6. STEM image of the catalyst after the reaction.

6. Hot filtration test and reuse experiments

Hot filtration test

After completing the reaction with La_2NiO_4 (La: 0.012 mmol), ethyl acetoacetate (78.1 mg, 0.60 mmol), and (*E*)-1-(4-fluorophenyl)but-2-en-1-one (118.2 mg, 0.72 mmol), the mixture was filtered through a PTFE syringe filter to remove the solid catalyst. The filtrate was extracted with *n*hexane in the same vial until no organic compounds were detectable by TLC. Subsequently, an additional portion of ethyl acetoacetate (78.1 mg, 0.60 mmol) and (*E*)-1-(4-fluorophenyl)but-2-en-1-one (118.2 mg, 0.72 mmol) were introduced into the remaining aqueous layer. The reaction and work-up were repeated under identical conditions, and the crude product was analyzed by ^{1}H NMR spectroscopy. The analysis confirmed that no further reaction had occurred, underscoring the absence of catalytic activity in the aqueous phase.

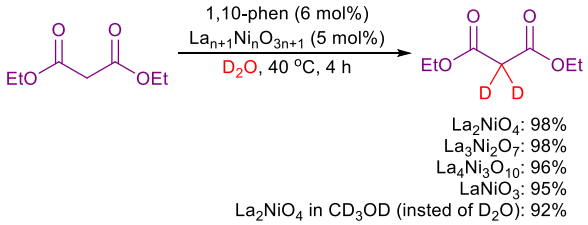
Reuse experiments

In a 6 mL vial equipped with a magnetic stirring bar, La_2NiO_4 (La: 0.06 mmol) was introduced under an inert atmosphere inside a glove box. Subsequently, (*E*)-1-(4-fluorophenyl)but-2-en-1-one (118.2 mg, 0.60 mmol), ethyl acetoacetate (78.1 mg, 0.72 mmol), and water (1.0 mL) were added. The vial was purged with argon, and the reaction mixture was stirred vigorously in a water bath maintained at 40 °C. After 30 minutes, *n*hexane was added to the vial, which was then vigorously shaken. The mixture was centrifuged at 3,500 rpm for 5 minutes, resulting in separation into a solid phase, an upper organic layer, and a lower aqueous layer. The organic layer was carefully collected using a pipette, ensuring that the solid catalyst remained undisturbed. This extraction process was repeated four times, after which the remaining aqueous phase and solid catalyst were used for the subsequent run. The combined organic extracts were concentrated under reduced pressure and dried in vacuo. The yield was determined by ^{1}H NMR spectroscopy using CH_2Br_2 as an internal standard.

1st run: 91% yield, 2nd run: >99% yield, 3rd run: >99% yield

7. Deuterium-labeling experiment

In a 2 mL vial equipped with a magnetic stirring bar, the mixed metal oxide catalyst (La: 0.030 mmol), previously stored under anaerobic conditions, was introduced inside a glove box. Subsequently, 1,10-phenanthroline monohydrate (7.14 mg, 0.036 mmol), diethyl malonate (96.1 mg, 0.60 mmol), and degassed deuterium oxide (D_2O, 1.0 mL) were added. The vial was purged with argon, and the reaction mixture was stirred vigorously in a water bath maintained at 40 °C. After 4 hours, $CDCl_3$ (0.5 mL) was added directly to the vial, and the mixture was vigorously shaken. The aqueous layer was carefully removed using a pipette. The remaining organic layer was passed through a PTFE syringe filter to remove the solid catalyst, and the filtrate was transferred to an NMR tube. The extent of deuterium incorporation was determined by ^1H NMR analysis.



Scheme S1. Deuterium-labeling experiment.

8. Reference

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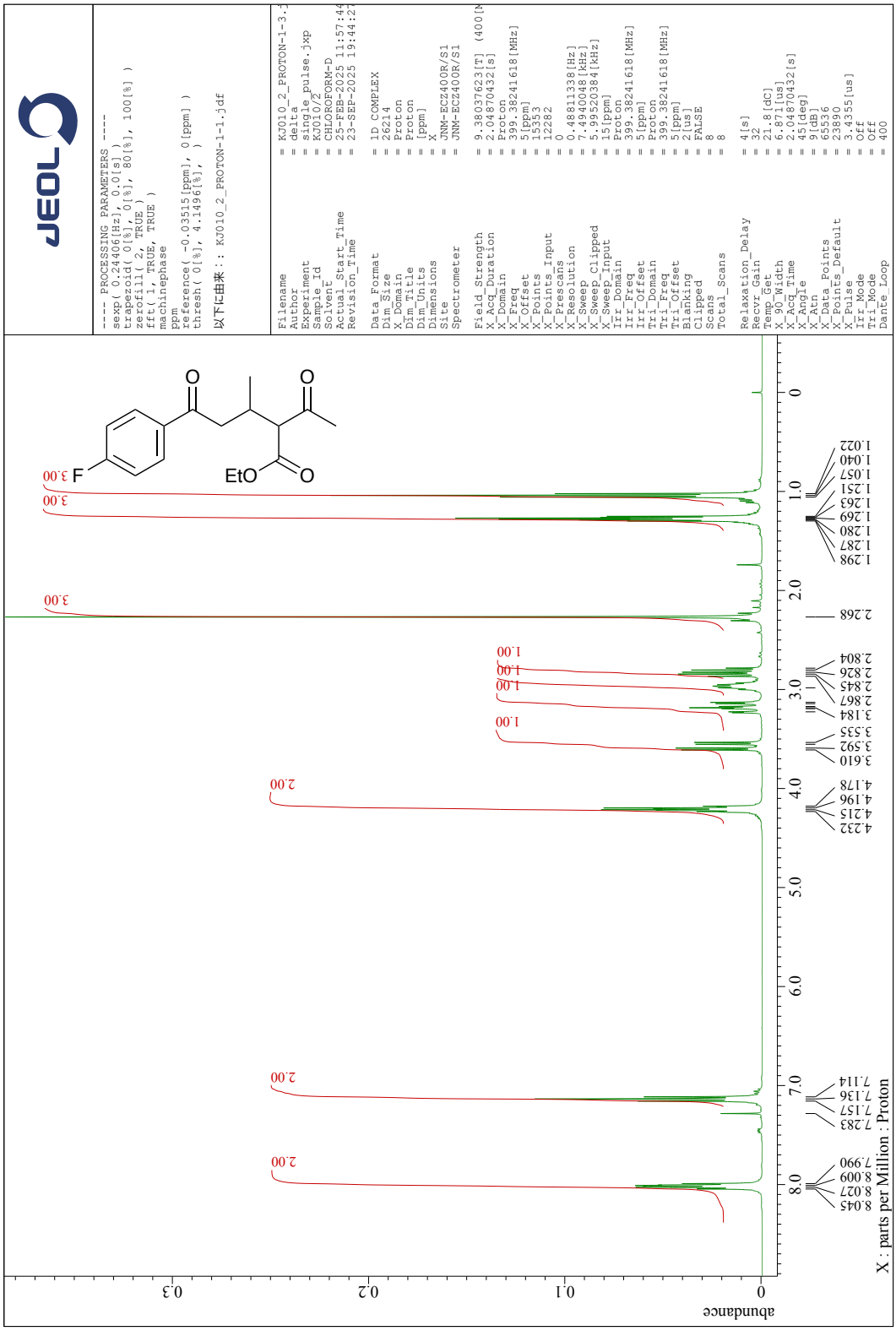
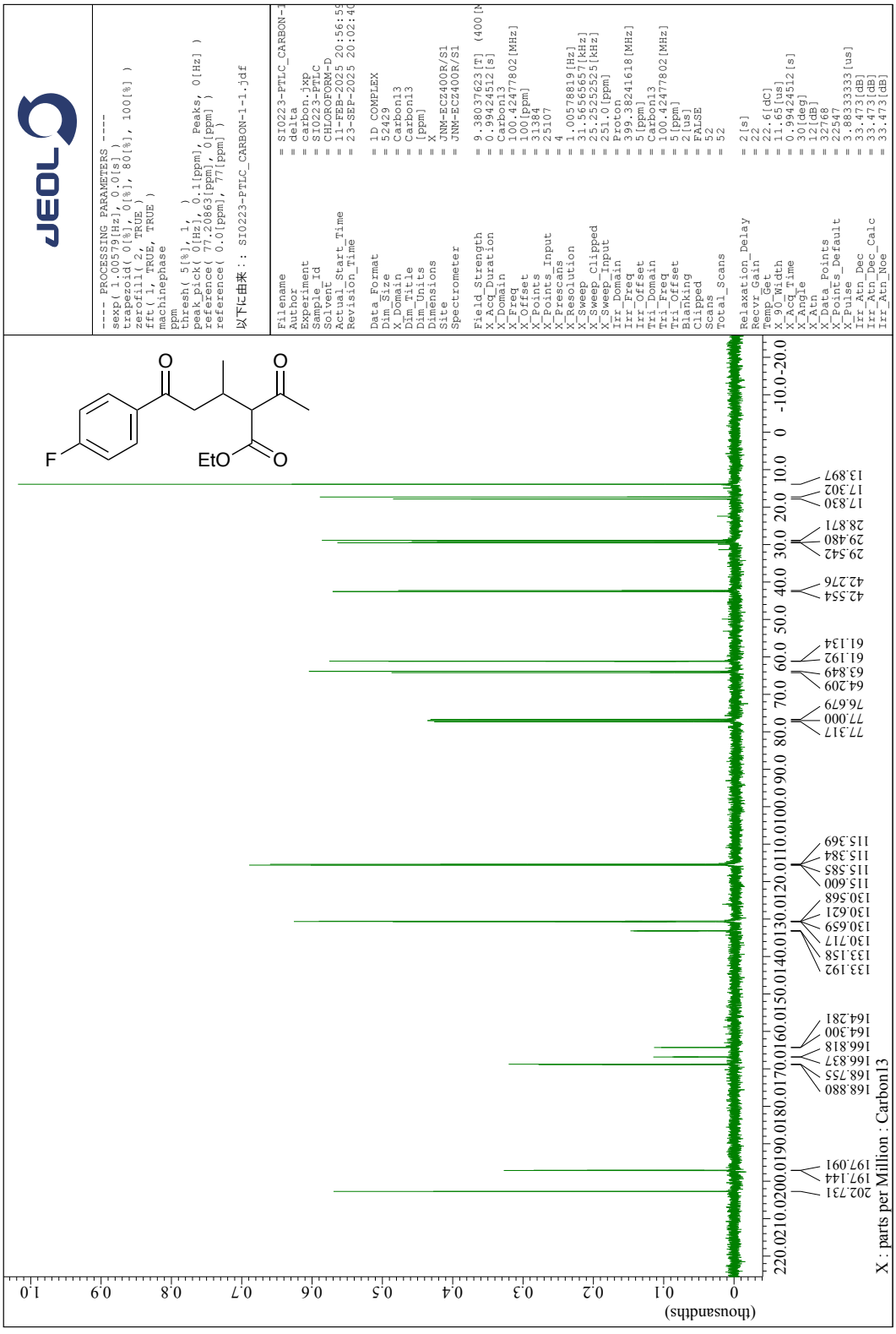
9. ^{1}H, ^{13}C & ^{19}F NMR spectra




JEOL
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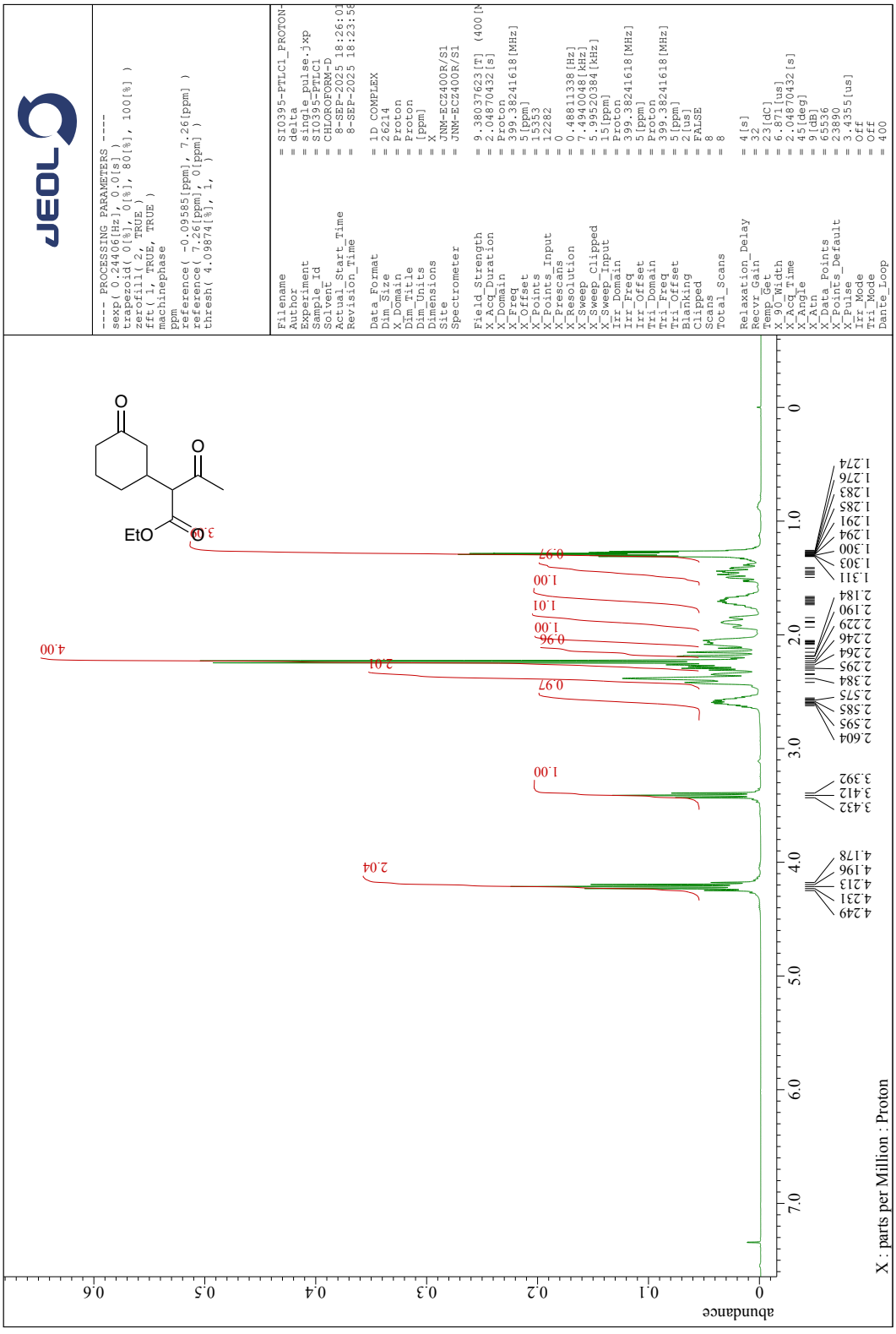
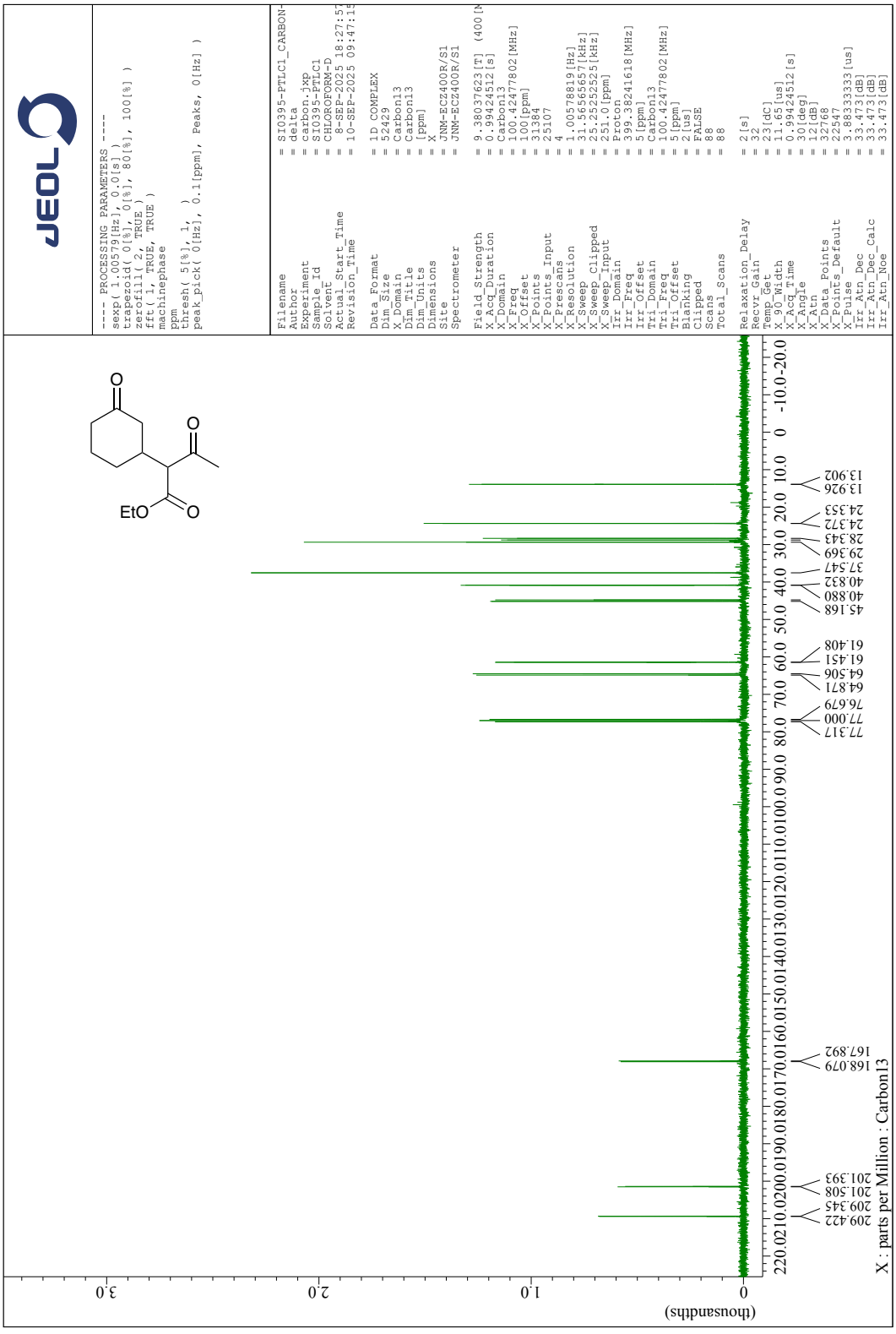
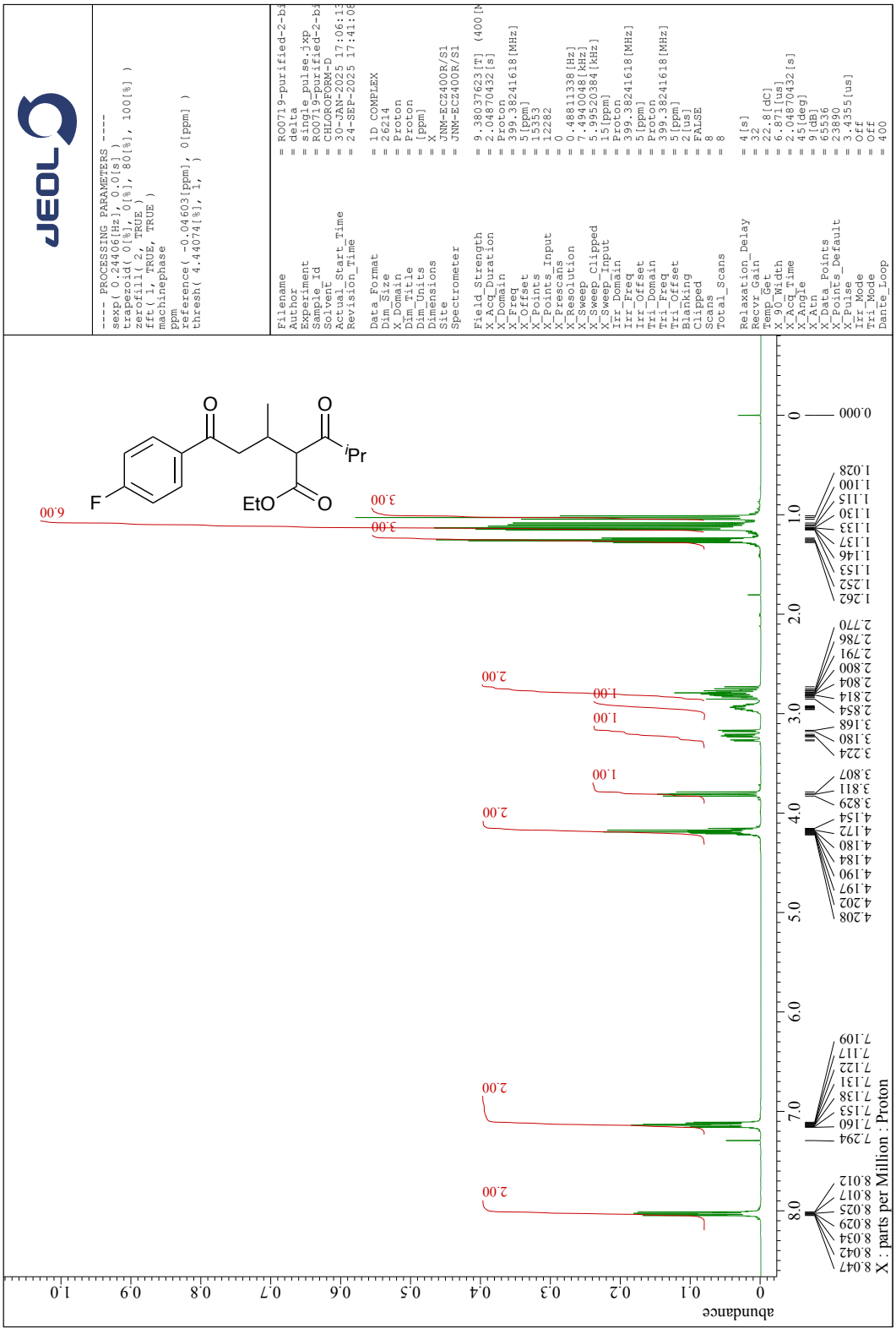
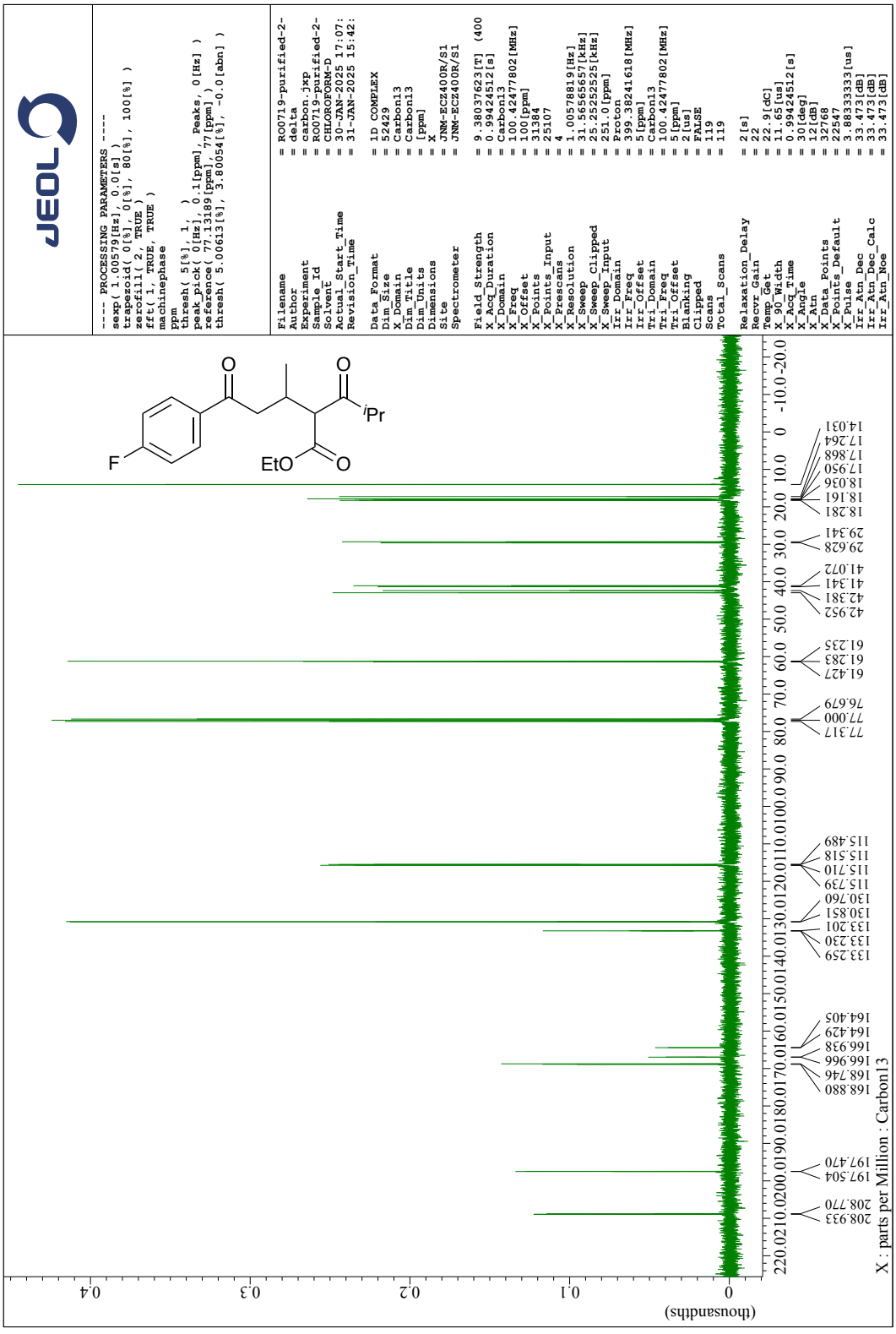
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.20863[ppm], 0[ppm])
reference(0.0[ppm], 77[ppm])
以下に由来：: SI0223-PTLC_CARBON-1-1.jdf
Filename = SI0223-PTLC_CARBON-1
Author = delta
Experiment = Carbon.jxp
Sample_Id = SI0223-PTLC
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-FEB-2025 20:56:59
Revision_Time = 23-SEP-2025 20:02:40
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 52
Total_Scans = 52
Relaxation_Delay = 2[s]
Recvr_Gain = 22
Temp_Get = 22.6[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Atn = 0[dB]
X_Data_Points = 12[dB]
X_Points_Default = 32768
X_Pulse = 3.88333333[us]
Ir_Atn_Dec = 33.473[dB]
Irr_Atn_Dec_Calc = 33.473[dB]
Irr_Atn_Noe = 33.473[dB]
O
O
F
EtO
O
(thousandths)
X : parts per Million : Carbon13
202.731
197.144
197.091
168.880
168.755
166.837
166.818
164.300
164.281
133.192
133.158
130.717
130.659
130.621
130.568
115.600
115.585
115.384
115.369
77.317
77.000
76.679
64.209
63.849
61.192
61.134
42.554
42.276
29.542
29.480
28.871
17.830
17.302
13.897

---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.89739[ppm], 77[ppm])
reference(77.31438[ppm], -63.72[ppm])
thresh(80.63702[%], 1)
reference(-63.72[ppm], -63.72[ppm])
reference(-63.72[ppm], -63.72[ppm])
reference(-63.72[ppm], -63.72[ppm])
reference(-64.3429[ppm], -63.72[ppm])
Filename = SI0223-PTLC_Fluorine
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0223-PTLC
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-FEB-2025 12:39:45
Revision_Time = 23-SEP-2025 20:08:48
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.0338032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.3[dC]
X_90_Width = 2.05[us]
X_Acq_Time = 2.0338032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
F
O
O
EtO
O
PhCF3
-106.233
-106.314
abundance
X : parts per Million : Fluorine19

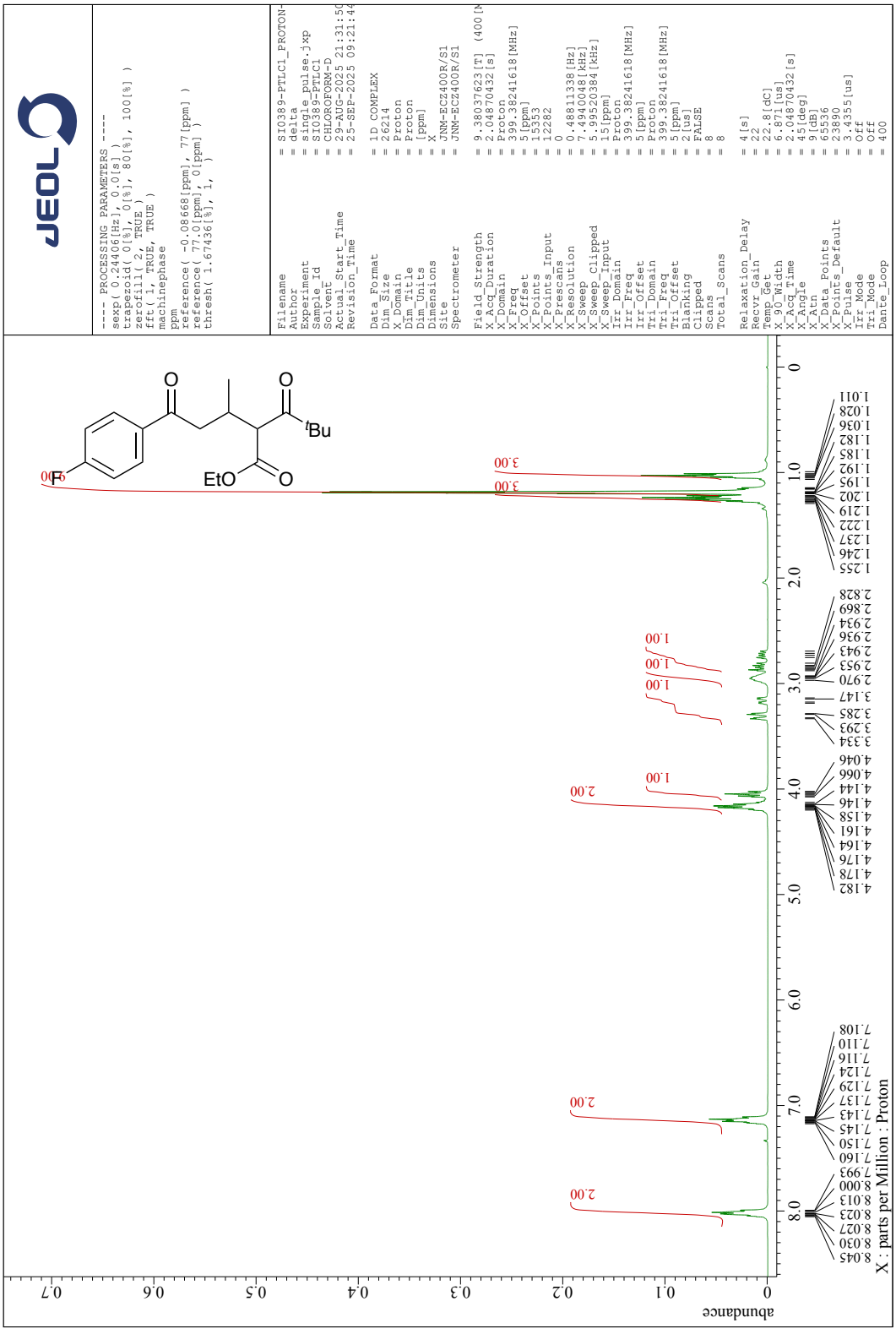

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.09585[ppm], 7.26[ppm])
reference(7.26[ppm], 0[ppm])
thresh(4.09874[%], 1,)
Filename = SI0395-PTLC1_PROTON-
Author = delta
Experiment = single_pulse.jxp
SampleId = SI0395-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-SEP-2025 18:26:01
Revision_Time = 8-SEP-2025 18:23:58
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 32
Temp_Get = 23.1[dC]
X_90_Width = 2.0417[us]
X_Acq_Time = 2.0487[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
abundance
X : parts per Million : Proton
EtO
4.00
2.01
0.97
1.00
2.04
1.00
0.97
1.01
1.00
0.96
3.00
4.249
4.231
4.213
4.196
4.178
3.432
3.412
3.392
2.604
2.595
2.585
2.575
2.384
2.295
2.264
2.246
2.229
2.190
2.184
1.311
1.303
1.300
1.294
1.291
1.285
1.283
1.276
1.274

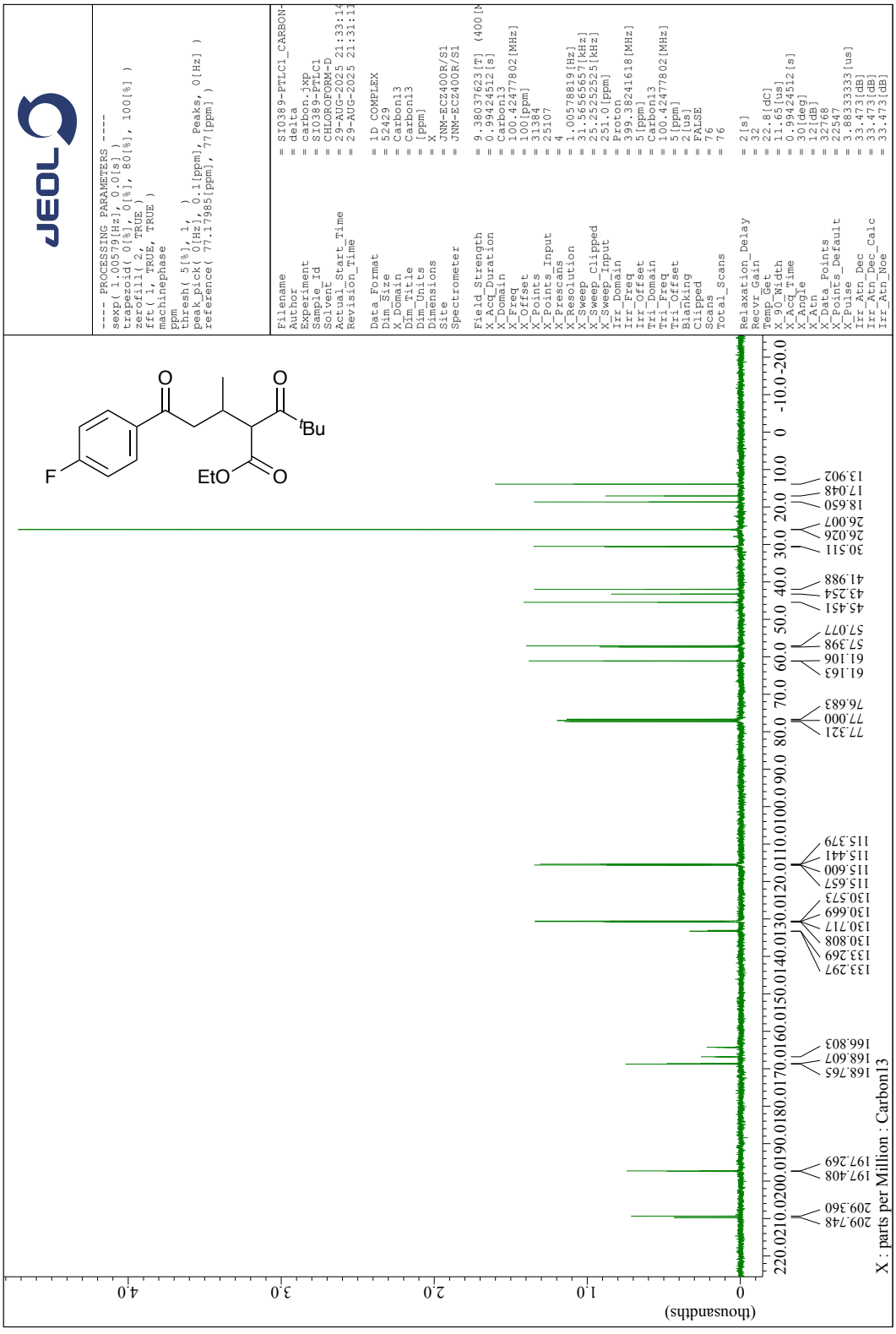

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
Filename = SI0395-PTLC1_CARBON-
Author = delta
Experiment = Carbon.jxp
Sample_Id = SI0395-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-SEP-2025 18:27:57
Revision_Time = 10-SEP-2025 09:47:15
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 88
Total_Scans = 88
Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Set = 31.1[dC]
X_90_Width = 21.65[us]
X_Acq_Time = 1.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Ir_Atn_Dec = 33.47[dB]
Ir_Atn_Dec_Calc = 33.47[dB]
Irr_Atn_Noe = 33.47[dB]
O
O
O
EtO
O
(thousandths)
3.0
2.0
1.0
0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
209.422
209.345
201.508
201.393
168.079
167.892
77.317
77.000
76.679
64.871
64.506
61.451
61.408
45.168
40.880
40.832
37.547
29.369
28.343
24.372
24.353
13.926
13.902


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.04603[ppm], 0[ppm])
thresh(4.44074[%], 1,)
Filename = RO0719-purified-2-b
Author = delta
Experiment = single_pulse.jxp
Sample_Id = RO0719-purified-2-b
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-JAN-2025 17:06:13
Revision_Time = 24-SEP-2025 17:41:08
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.8[dC]
X_90_Width = 2.6875[us]
X_Acq_Time = 2.04870432[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
F
O
O
O
EtO
O
iPr
6.00
3.00
3.00
2.00
2.00
1.00
1.00
2.00
2.00
abundance
X : parts per Million : Proton

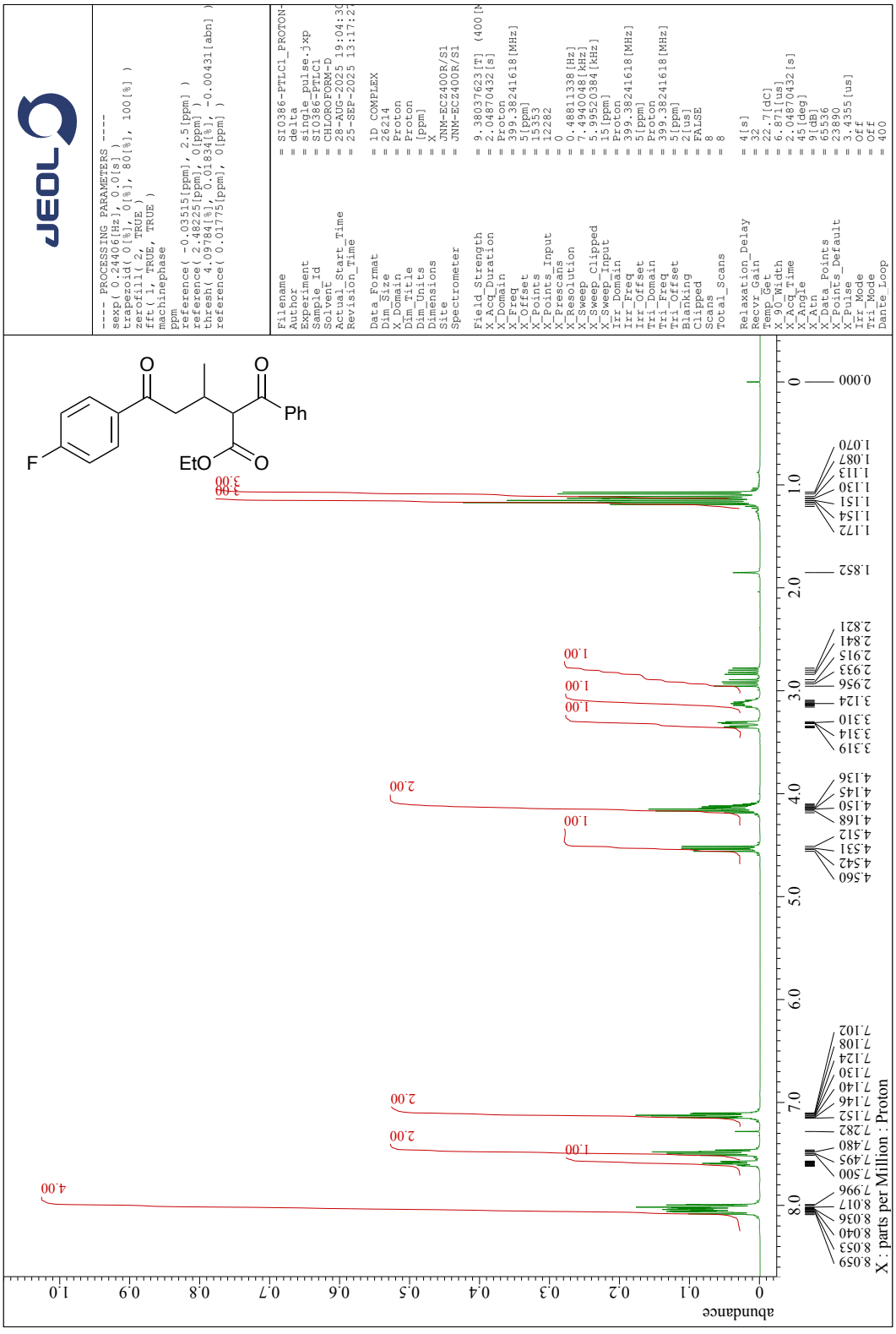

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.13189[ppm], 77[ppm])
thresh(5.00613[%], 3.80054[%], -0.0[abn])
Filename = RO0719-purified-2-
Author = delta
Experiment = carbon.jxp
Sample_Id = RO0719-purified-2-
SolventE = CHLOROFORM-D
Actual_Start_Time = 30-JAN-2025 17:07:
Revision_Time = 31-JAN-2025 15:42:
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
DIm_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 119
Total_Scans = 119
Relaxation_Delay = 2[s]
Recvr_Gain = 22
Temp_Get = 22.9[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Irr_Atn_Dec = 33.473[dB]
Irr_Atn_Dec_Calc = 33.473[dB]
Irr_Atn_Noe = 33.473[dB]
O
O
iPr
F
EtO
O
(thousandths)
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13
208.933
208.770
197.504
197.470
168.880
168.746
166.966
166.938
164.429
164.405
133.259
133.230
133.201
130.851
130.760
115.739
115.710
115.518
115.489
77.317
77.000
76.679
61.427
61.283
61.235
42.952
42.381
41.341
41.072
29.628
29.341
18.281
18.161
18.036
17.950
17.868
17.264
14.031

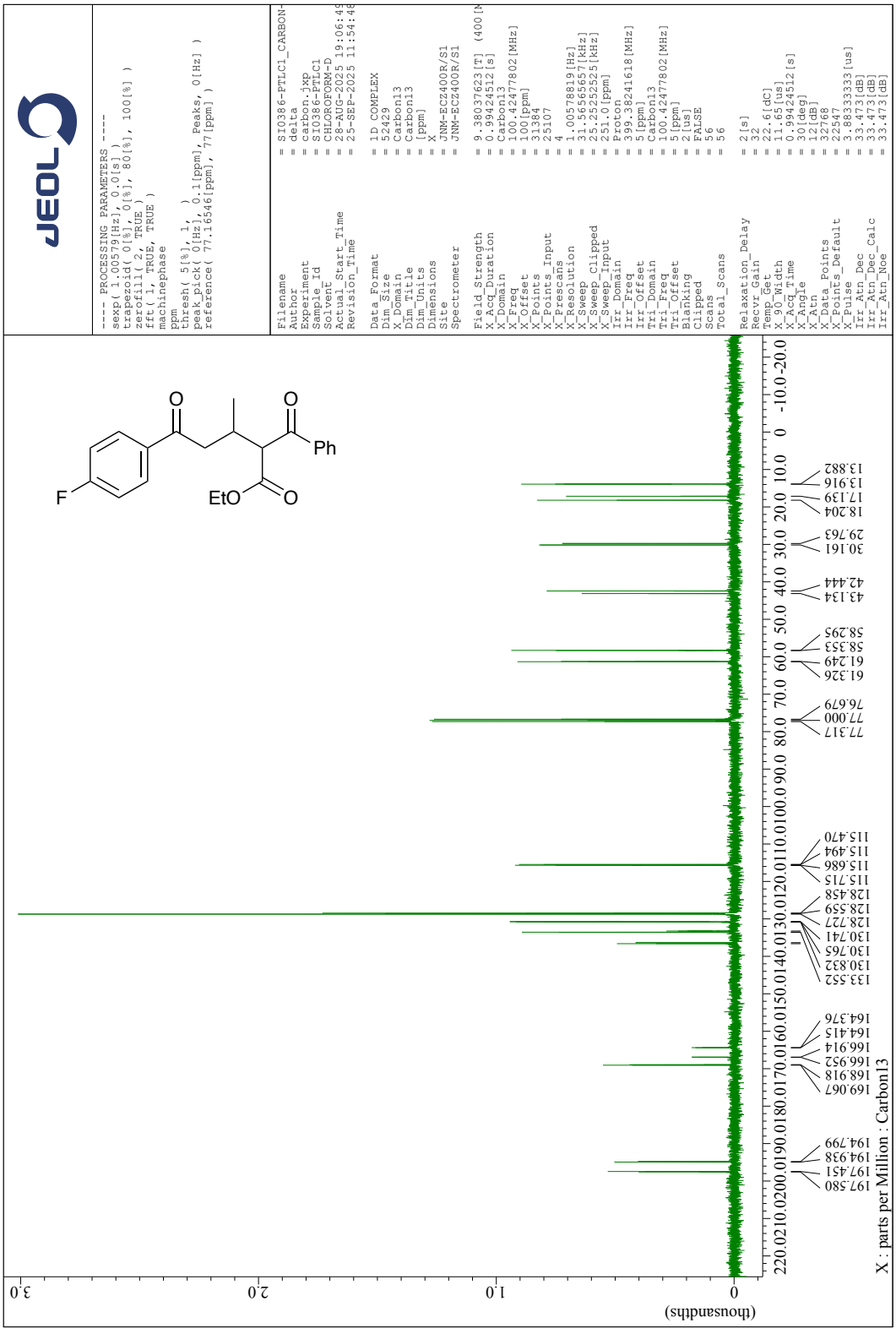
---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz] 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.63544[ppm], -63.72[ppm])
thresh(85.8309[%], 1)
以下に由来:: RO0719-purified-2-big_Fluorine-1-1.
Filename = RO0719-purified-2-
Author = delta
Experiment = single pulse jxp
Sample_Id = RO0719-purified-2-
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-JAN-2025 17:24:
Revision_Time = 31-JAN-2025 15:44:
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400
X_Acq_Duration = 2.03380032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.9[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 2.0338032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
F
O
O
EtO
O
iPr
PhCF3
-106.220
-106.320
abundance
0.6
0.5
0.4
0.3
0.2
0.1
0
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
X : parts per Million : Fluorine19


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.08668[ppm], 77[ppm])
reference(77.0[ppm], 0[ppm])
thresh(1.67436[%], 1,)
Filename = SI0389-PTLC1_PROTON-
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0389-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-AUG-2025 21:31:50
Revision_Time = 25-SEP-2025 09:21:44
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.8[dC]
X_90_Width = 6.87[us]
X_Acq_Time = 2.04870432[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
O
tBu
EtO
O
F
3.00
3.00
2.00
2.00
2.00
1.00
1.00
1.00
abundance
X : parts per Million : Proton

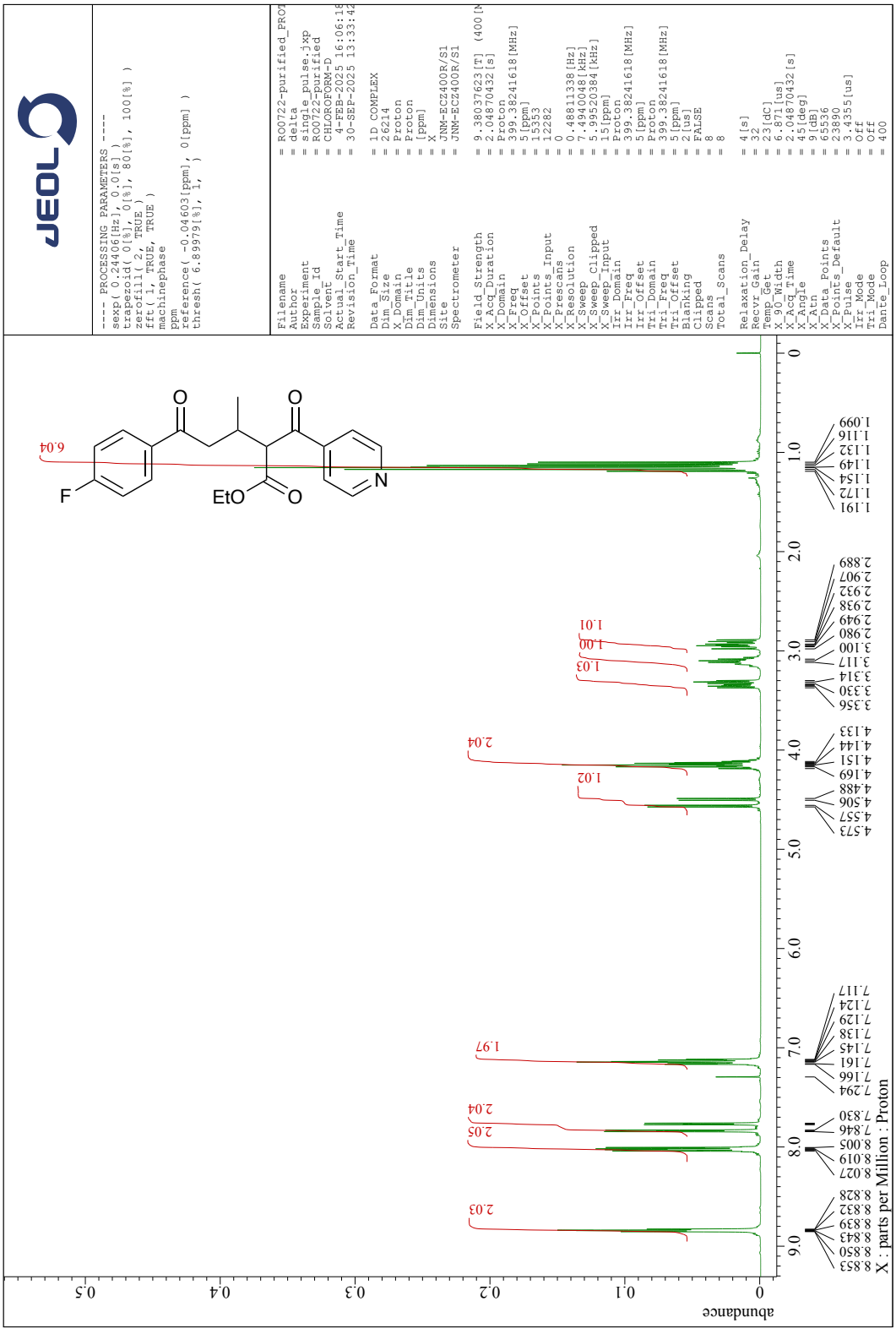

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.17985[ppm], 77[ppm])
Filename = SI0389-PTLC1_CARBON-
Author = delta
Experiment = Carbon.jxp
Sample_Id = SI0389-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-AUG-2025 21:33:14
Revision_Time = 29-AUG-2025 21:31:11
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 76
Total_Scans = 76
Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Get = 22.8[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Atn = 10[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Ir_Atn_Dec = 33.47[dB]
Irr_Atn_Dec_Calc = 33.47[dB]
Irr_Atn_Noe = 33.47[dB]
O
O
tBu
F
EtO
O
(thousandths)
X : parts per Million : Carbon13
209.748
209.360
197.408
197.269
168.765
168.607
166.803
133.297
133.269
130.808
130.717
130.669
130.573
115.657
115.600
115.441
115.379
77.321
77.000
76.683
61.163
61.106
57.398
57.077
45.451
43.254
41.988
30.511
26.026
26.007
18.650
17.048
13.902

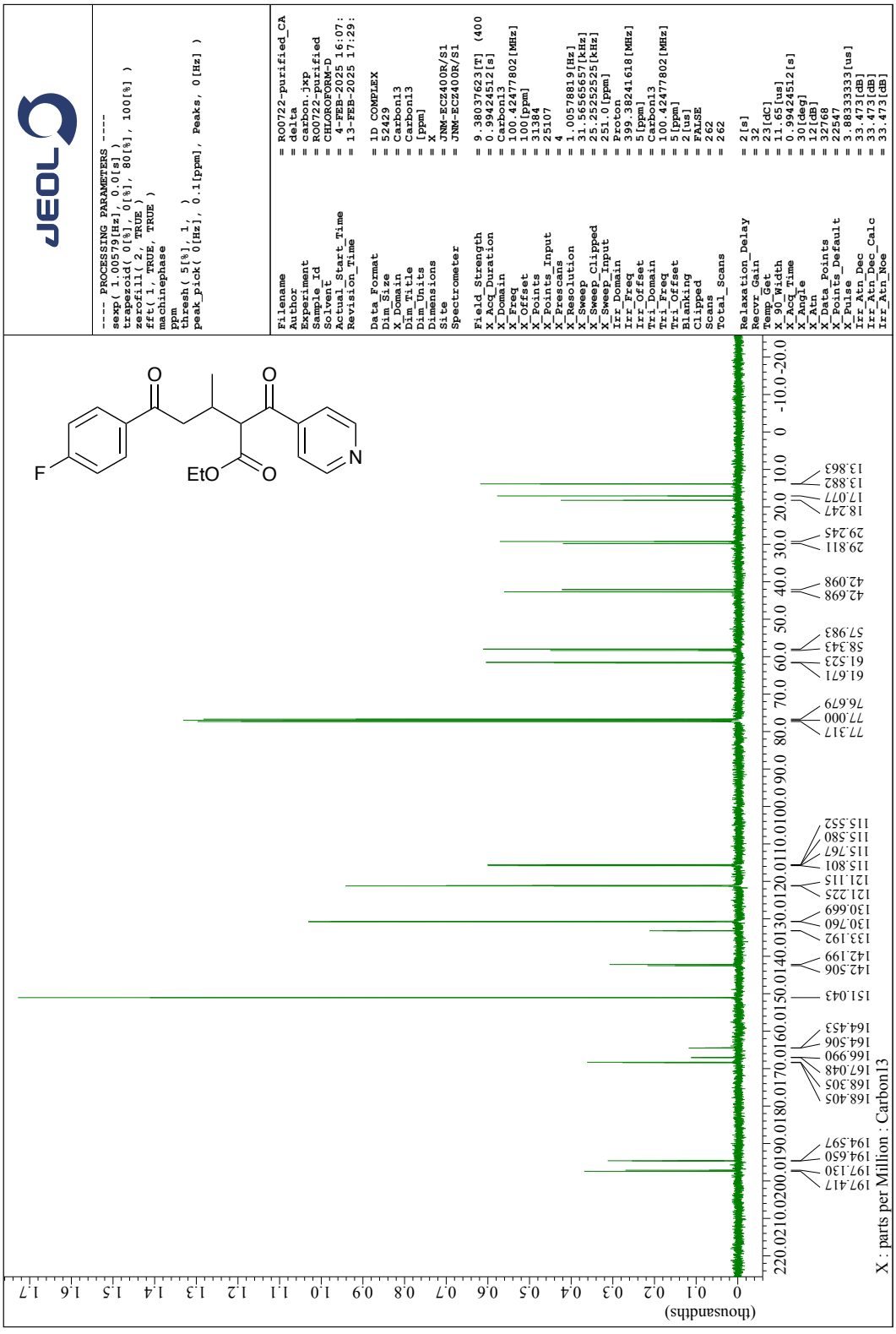
JEOL
---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.62535[ppm], -63.72[ppm])
thresh(61.77718[%], 1,)
Filename = SI0389-PTLC1_Fluorin
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0389-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-AUG-2025 22:23:16
Revision_Time = 25-SEP-2025 09:23:48
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.03380032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.9[dC]
X_90_Width = 2.05[us]
X_Acq_Time = 2.0338032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Ir_Mode = Off
Tri_Mode = Off
Date_Loop = 400
O
O
tBu
F
EtO
O
PhCF3
-106.257
-106.466
abundance
0
0.1
0.2
0.3
0.4
0.5
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
X : parts per Million : Fluorine19


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.01[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.03515[ppm], 2.5[ppm])
reference(2.48225[ppm], 0[ppm])
thresh(4.09784[%], 0.01834[%], -0.00431[abn])
reference(0.01775[ppm], 0[ppm])
Filename = SI0386-PTLC1_PROTON-
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0386-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-AUG-2025 19:04:3
Revision_Time = 25-SEP-2025 13:17:2
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.7[dC]
X_90_Width = 6.8711[us]
X_Acq_Time = 2.0487[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
Ph
F
EtO
O
4.00
2.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
3.00
3.00
abundance
X : parts per Million : Proton

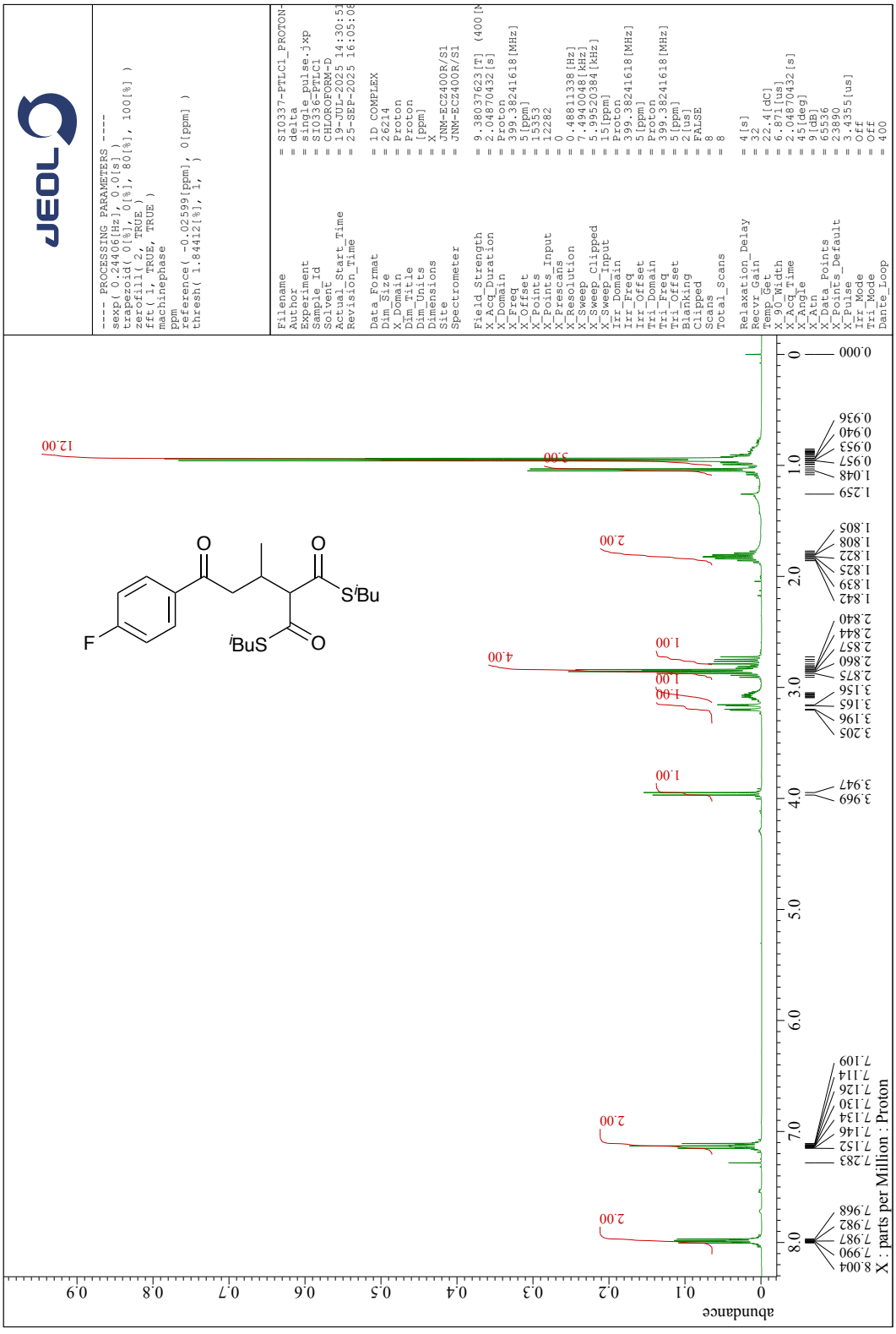

JEOL
--- PROCESSING PARAMETERS ---
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.16546[ppm], 77[ppm])
Filename = SI0386-PTLC1_CARBON-
Author = delta
Experiment = Carbon.jxp
Sample_Id = SI0386-PTLC1
SolventE = CHLOROFORM-D
Actual_Start_Time = 28-AUG-2025 19:06:49
Revision_Time = 25-SEP-2025 11:54:48
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 56
Total_Scans = 56
Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Get = 22.6[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Atn = 0[dB]
X_Atn_Dec = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Ir_Atn_Dec = 33.47[dB]
Irr_Atn_Dec_Calc = 33.47[dB]
Irr_Atn_Noe = 33.47[dB]
O
O
Ph
F
EtO
O
(thousandths)
3.0
2.0
1.0
0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
197.580
197.451
194.938
194.799
169.067
168.918
166.952
166.914
164.415
164.376
133.552
130.832
130.765
130.741
128.727
128.559
128.458
115.715
115.686
115.494
115.470
77.317
77.000
76.679
61.326
61.249
58.353
58.295
43.134
42.444
30.161
29.763
18.204
17.139
13.916
13.882

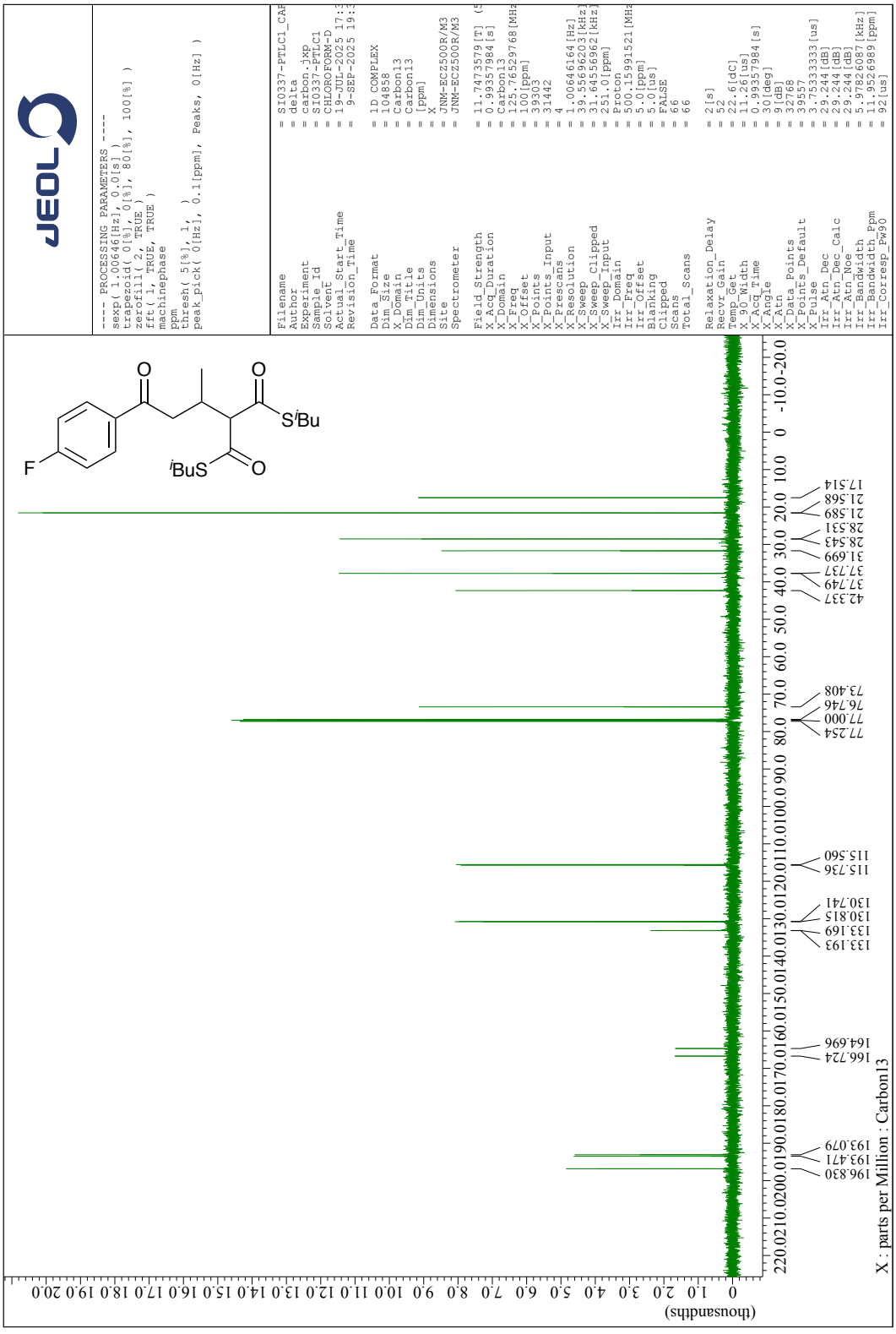
JEOL
---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.58257[ppm], -63.72[ppm])
thresh(74.52637[%], 1,)
Filename = SI0386-PTLC1_Fluorir
Author = delta
Experiment = single pulse.jxp
Sample_Id = SI0386-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-AUG-2025 20:49:48
Revision_Time = 25-SEP-2025 11:52:44
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.03380032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.9[dC]
X_90_Width = 2.05[us]
X_Acq_Time = 2.0338032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
Ph
F
EtO
O
PhCF3
-106.191
-106.315
abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
X : parts per Million : Fluorine19


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.04603[ppm], 0[ppm])
thresh(6.89979[%], 1,)
Filename = RO0722-purified_PROT
Author = delta
Experiment = single_pulse.jxp
Sample_Id = RO0722-purified
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-FEB-2025 16:06:18
Revision_Time = 30-SEP-2025 13:33:44
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 32
Temp_Get = 23[dC]
X_90_Width = 8.25[us]
X_Acq_Time = 2.0487[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
abundance
X : parts per Million : Proton
6.04
F
EtO
O
N
2.03
2.04
2.05
1.97
1.02
2.04
1.03
1.00
1.01

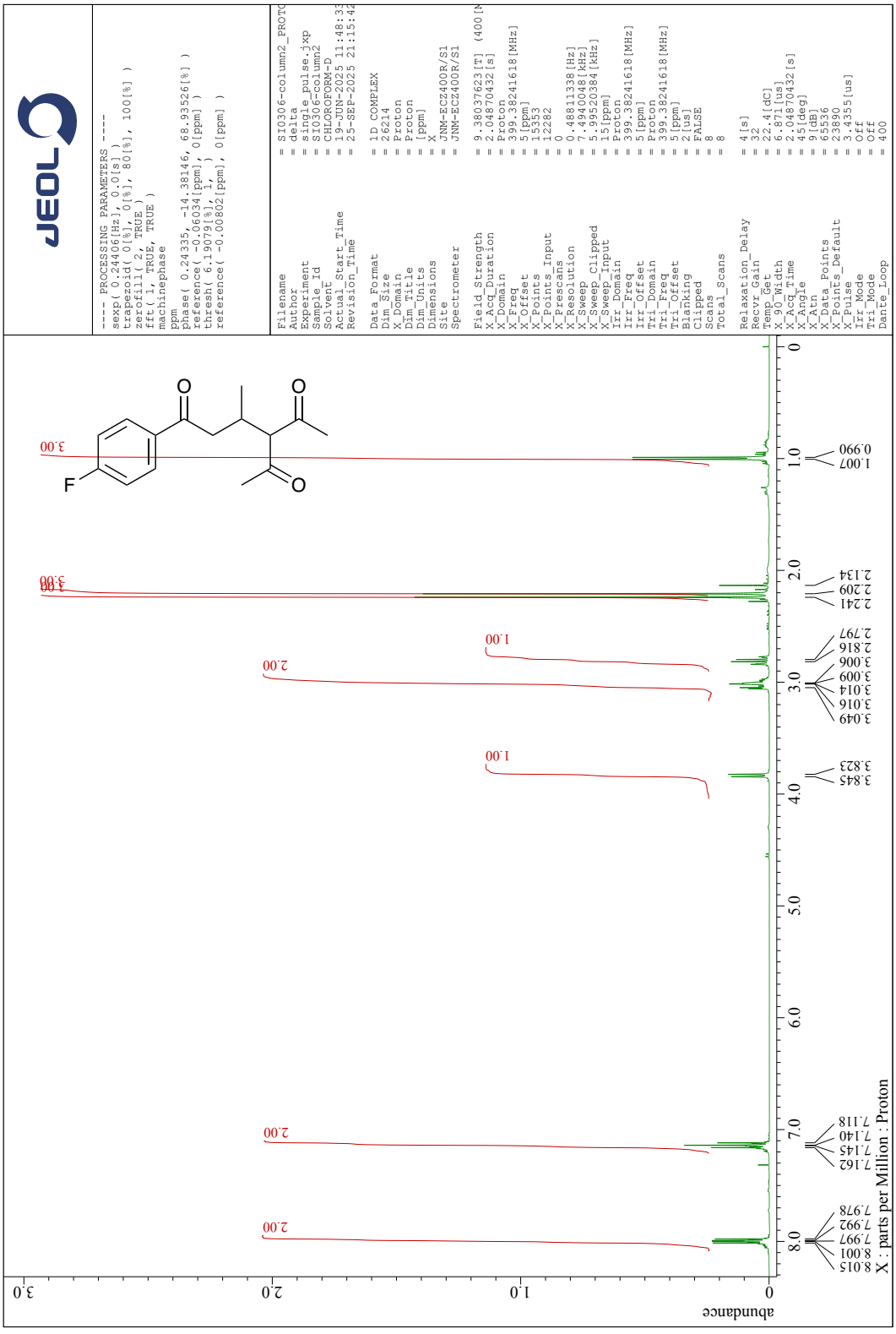

JEOL
--- PROCESSING PARAMETERS ---
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
Filename = RO0722-purified_CA
Author = delta
Experiment = carbon.jxp
Sample_Id = RO0722-purified
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-FEB-2025 16:07:
Revision_Time = 13-FEB-2025 17:29:
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 262
Total_Scans = 262
Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Set = 23[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Irr_Atn_Dec = 33.473[dB]
Irr_Atn_Dec_Calc = 33.473[dB]
Irr_Atn_Noe = 33.473[dB]
O
O
F
EtO
O
N
(thousandths)
X : parts per Million : Carbon13
197.417
197.130
194.650
194.597
168.405
168.305
167.048
166.990
164.506
164.453
151.043
142.506
142.199
133.192
130.760
130.669
121.225
121.115
115.801
115.767
115.580
115.552
77.317
77.000
76.679
61.671
61.523
58.343
57.983
42.698
42.098
29.811
29.245
18.247
17.077
13.882
13.863

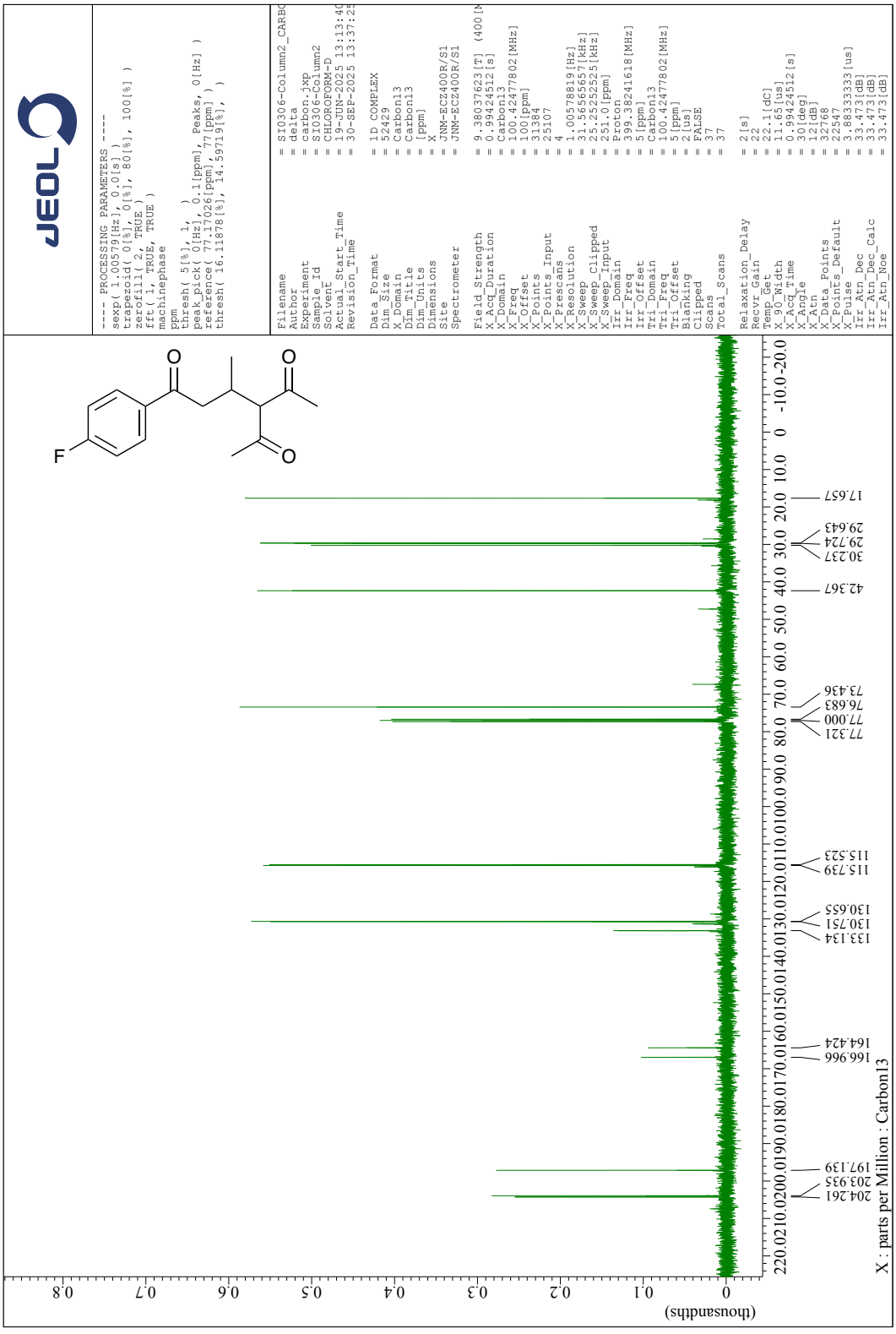
JEOL
---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.59507[ppm], -63.72[ppm])
reference(-63.72[ppm], -63.72[ppm])
thresh(68.12692[%], 0.08533[%], 0.00347[abn]
Filename = RO0722-purified-2_
Author = delta
Experiment = single pulse jmp
Sample_Id = RO0722-purified-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-FEB-2025 17:10:
Revision_Time = 5-FEB-2025 17:09:
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400
X_Acq_Duration = 2.03380032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.9[dC]
X_90_Width = 2.5[us]
X_Acq_Time = 2.03380032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
F
O
O
EtO
O
N
PhCF3
-105.862
-106.048
abundance
0
0.1
0.2
0.3
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
X : parts per Million : Fluorine19


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.02599[ppm], 0[ppm])
thresh(1.84412[%], 1,)
Filename = SI0337-PTLC1_PROTON-
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0336-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUL-2025 14:30:51
Revision_Time = 25-SEP-2025 16:05:08
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22.4[dC]
Temp_Get = 22.1[deg]
X_90_Width = 2.04870432[s]
X_Acq_Time = 45[deg]
X_Angle = 9[dB]
X_Atn = 65536
X_Data_Points = 23890
X_Points_Default = 3.4355[us]
X_Pulse = Off
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
S^{i}Bu
F
^{i}BuS
O
12.00
5.00
4.00
2.00
2.00
2.00
1.00
1.00
1.00
1.00
abundance
X : parts per Million : Proton
8.004
7.990
7.987
7.982
7.968
7.283
7.152
7.146
7.134
7.130
7.126
7.114
7.109
3.969
3.947
3.205
3.196
3.165
3.156
2.875
2.860
2.857
2.844
2.840
1.842
1.839
1.825
1.822
1.808
1.805
1.259
1.048
0.957
0.953
0.940
0.936
0.000

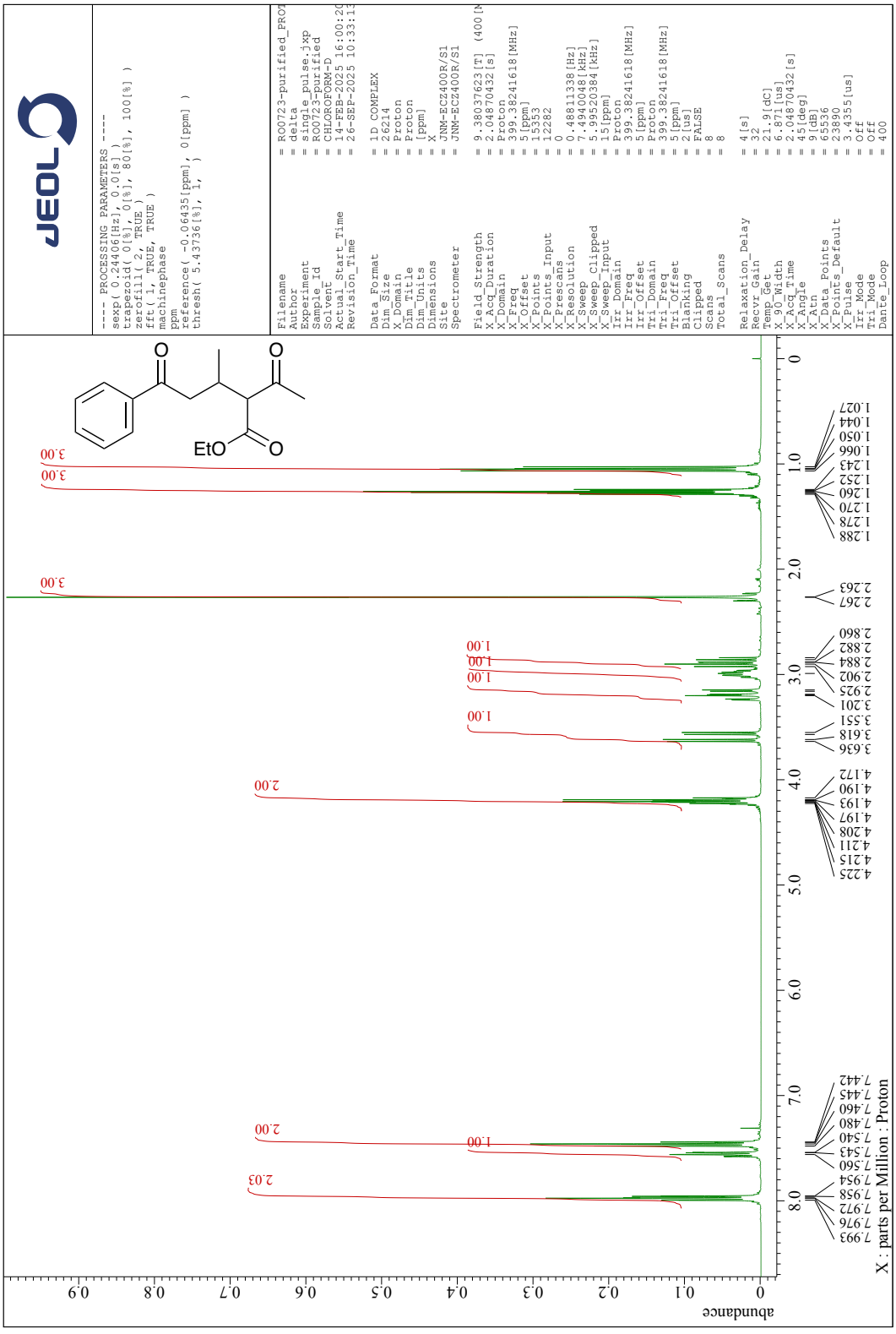

JEOL
--- PROCESSING PARAMETERS ---
sexp(1.00646[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
Filename = ST0337-PTLC1_CAR
Author = delta
Experiment = carbon.jxp
SampleId = ST0337-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUL-2025 17:3
Revision_Time = 9-SEP-2025 19:3
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.7473579[T] (5
X_Acq_Duration = 0.99357984[s]
X_Domain = Carbon13
X_Freq = 125.765297.68[MHz
X_Offset = 100[ppm]
X_Points = 39303
X_Points_Input = 31442
X_Prescans = 4
X_Resolution = 1.00646164[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 66
Total_Scans = 66
Relaxation_Delay = 2[s]
Recvr_Gain = 52
Temp_Get = 22.6[dC]
X_90_Width = 11.66[us]
X_Acq_Time = 0.99357984[s]
X_Angle = 90[deg]
X_Atn = 32[dB]
X_Data_Points = 39557
X_Points_Default = 3.75333333[us]
Irr_Atn_Dec = 29.244[dB]
Irr_Atn_Dec_Calc = 29.244[dB]
Irr_Atn_Noe = 29.244[dB]
Irr_Bandwidth = 5.97826087[kHz]
Irr_Bandwidth_Ppm = 11.9526989[ppm]
Irr_Corresp_Pw90 = 92[us]
O
O
S^{i}Bu
F
^{i}BuS
O
196.830
193.471
193.079
166.724
164.696
133.193
133.169
130.815
130.741
115.736
115.560
77.254
77.000
76.746
73.408
42.337
37.749
37.737
31.699
28.543
28.531
21.589
21.568
17.514
(thousandths)
X : parts per Million : Carbon13

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.59891[ppm], -63.72[ppm])
thresh(99.86521[%], 1,)
Filename = SI0337-PTLC1_Fluorin
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0337-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUL-2025 18:13:39
Revision_Time = 25-SEP-2025 21:34:54
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.03380032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.8[dC]
X_90_Width = 2.03[us]
X_Acq_Time = 2.033380032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Ir_Mode = Off
Tri_Mode = Off
Date_Loop = 400
F
O
O
S^{i}Bu
^{i}BuS
O
PhCF$_3$
-106.130
abundance
0
0.1
0.2
0.3
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
X : parts per Million : Fluorine19

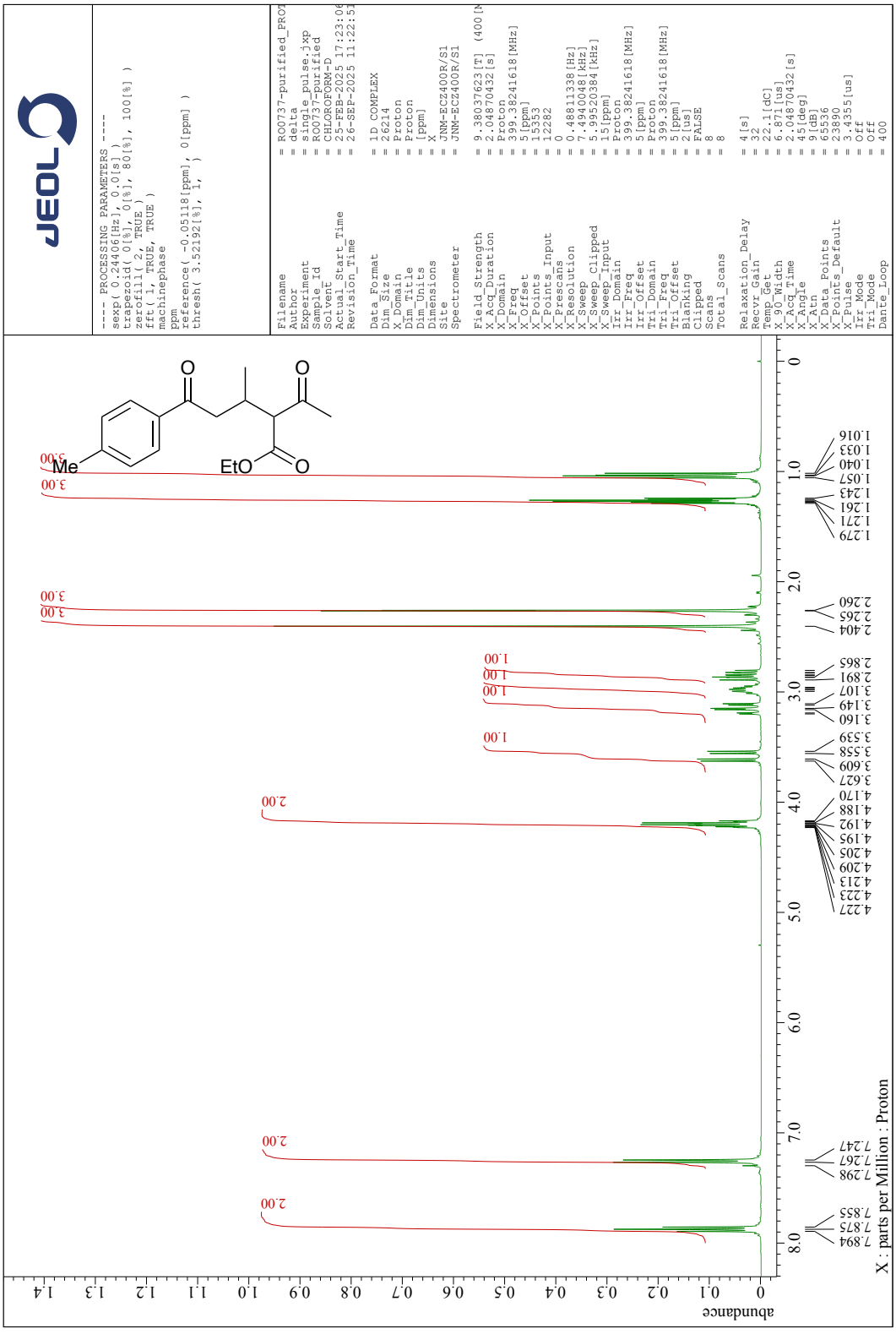

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(0.24335, -14.38146, 68.93526[%])
reference(-0.06034[ppm], 0[ppm])
thresh(6.19079[%], 1)
reference(-0.00802[ppm], 0[ppm])
Filename = SI0306-column2_PROTC
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0306-column2
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2025 11:48:33
Revision_Time = 25-SEP-2025 21:15:44
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22.4[dC]
Temp_Get = 22.1[deg]
X_90_Width = 2.0487[us]
X_Acq_Time = 2.04870432[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Ir_Mode = Off
Tri_Mode = Off
Date_Loop = 400
O
O
O
F
3.00
2.00
2.00
2.00
1.00
1.00
1.007
0.990
2.241
2.209
2.134
3.049
3.016
3.014
3.009
3.006
2.816
2.797
3.845
3.823
7.162
7.145
7.140
7.118
8.015
8.001
7.997
7.992
7.978
abundance
X : parts per Million : Proton

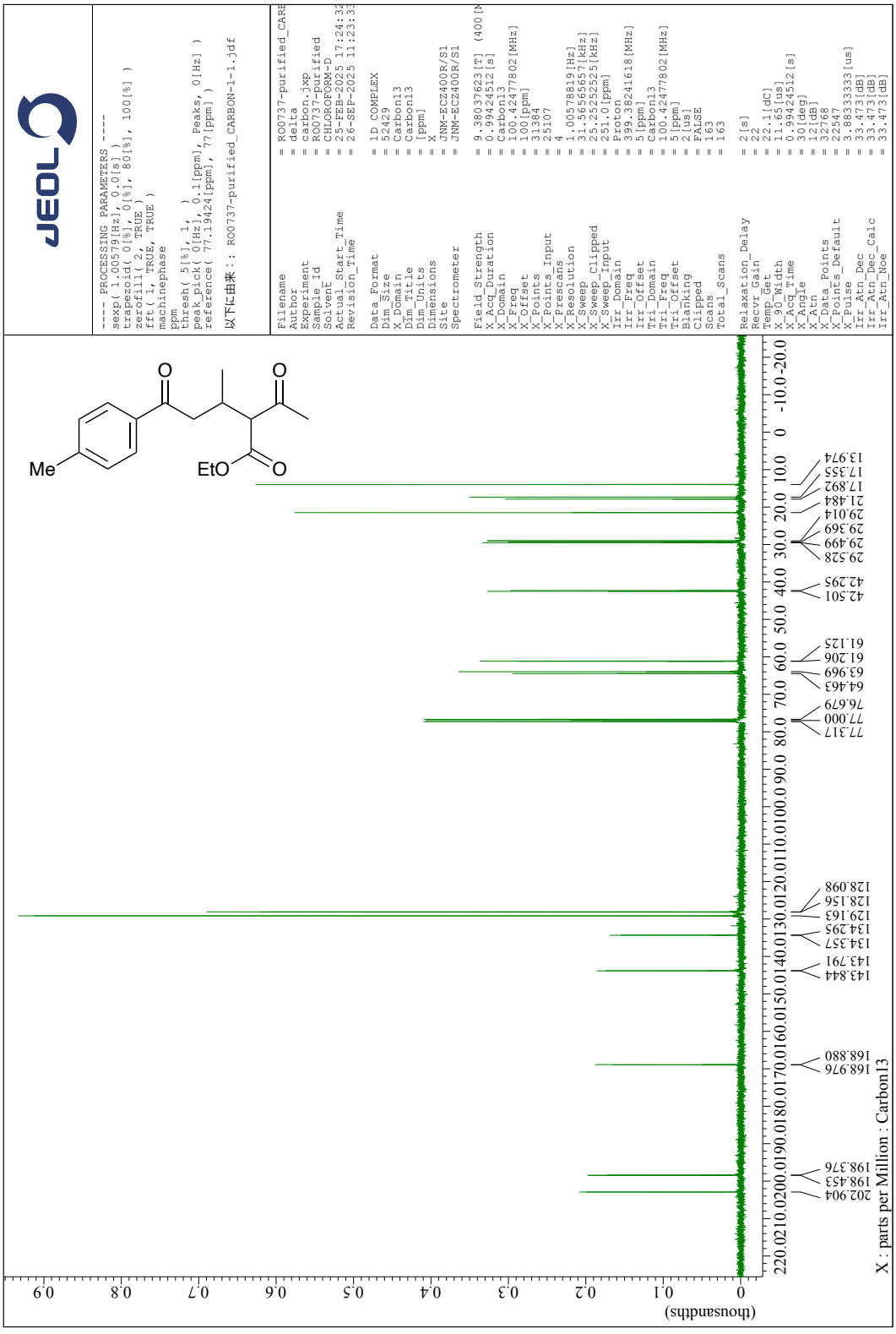

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.170260[ppm], 77[ppm])
thresh(16.118780[%], 14.597190[%],)
Filename = SI0306-Column2_CARBO
Author = delta
Experiment = Carbon.jxp
Sample_Id = SI0306-Column2
SolvenT = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2025 13:13:40
Revision_Time = 30-SEP-2025 13:37:28
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
DIm_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 37
Total_Scans = 37
Relaxation_Delay = 2[s]
Recvr_Gain = 22
Temp_Get = 22.1[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Irr_Atn_Dec = 33.47[dB]
Irr_Atn_Dec_Calc = 33.47[dB]
Irr_Atn_Noe = 33.47[dB]
O
O
O
F
(thousandths)
X : parts per Million : Carbon13
204.261
203.935
197.139
166.966
164.424
133.134
130.751
130.655
115.739
115.523
77.321
77.000
76.683
73.436
42.367
30.237
29.724
29.643
17.657

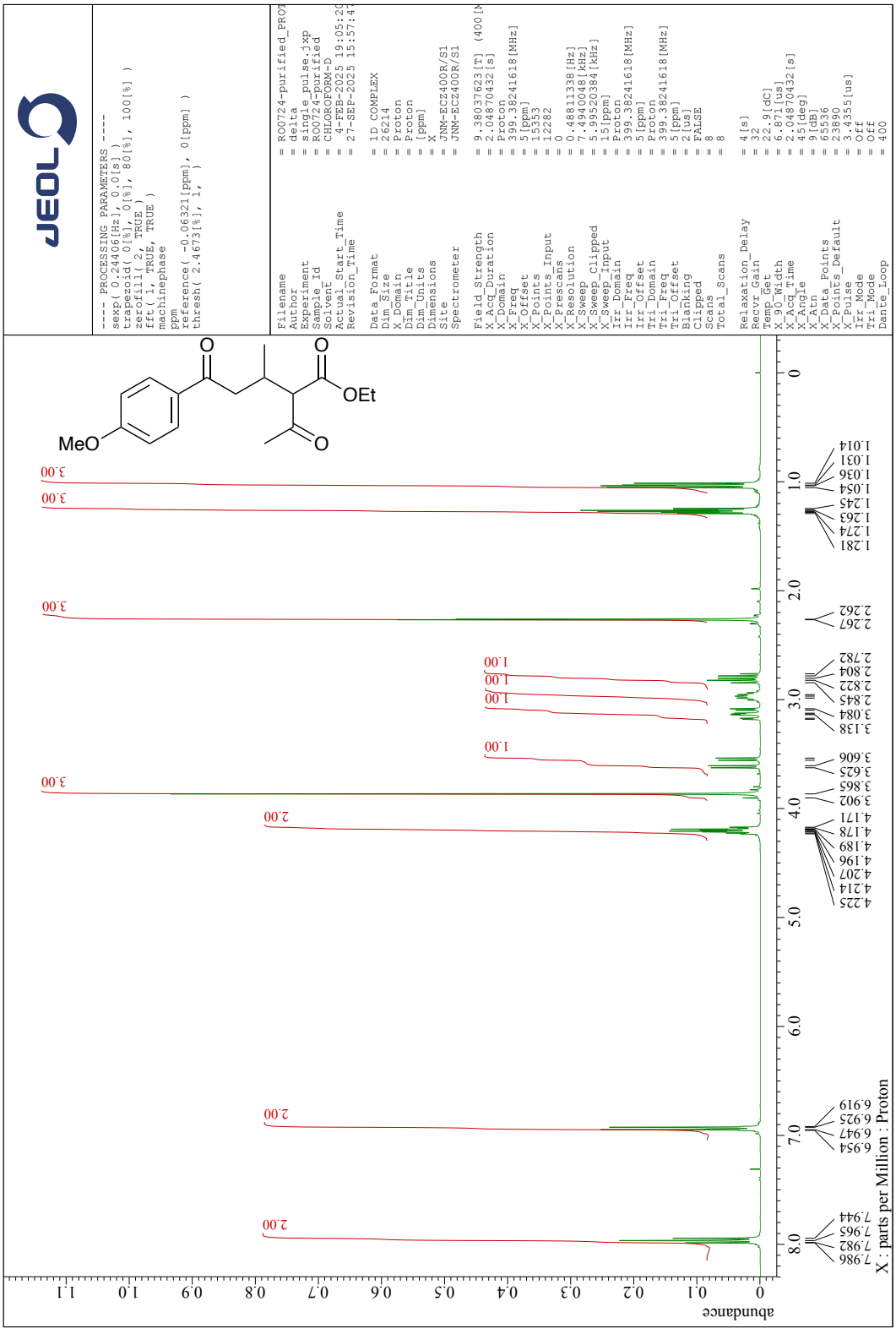
---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(55.75883[%], 0.04785[%], -0.00586[abn]
reference(-62.58017[ppm], -63.72[ppm])
以下に由来：: SI0306-Column_Fluorine-1-1.jdf
Filename = SI0306-Column_Fluori
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0306-Column
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-JUN-2025 19:08:04
Revision_Time = 25-SEP-2025 17:32:18
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.0338032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.6[dC]
X_90_Width = 2.03[us]
X_Acq_Time = 2.0338032[s]
X_Atn = 45[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
O
F
PhCF3
-106.032
-106.047
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-190.0
X : parts per Million : Fluorine19

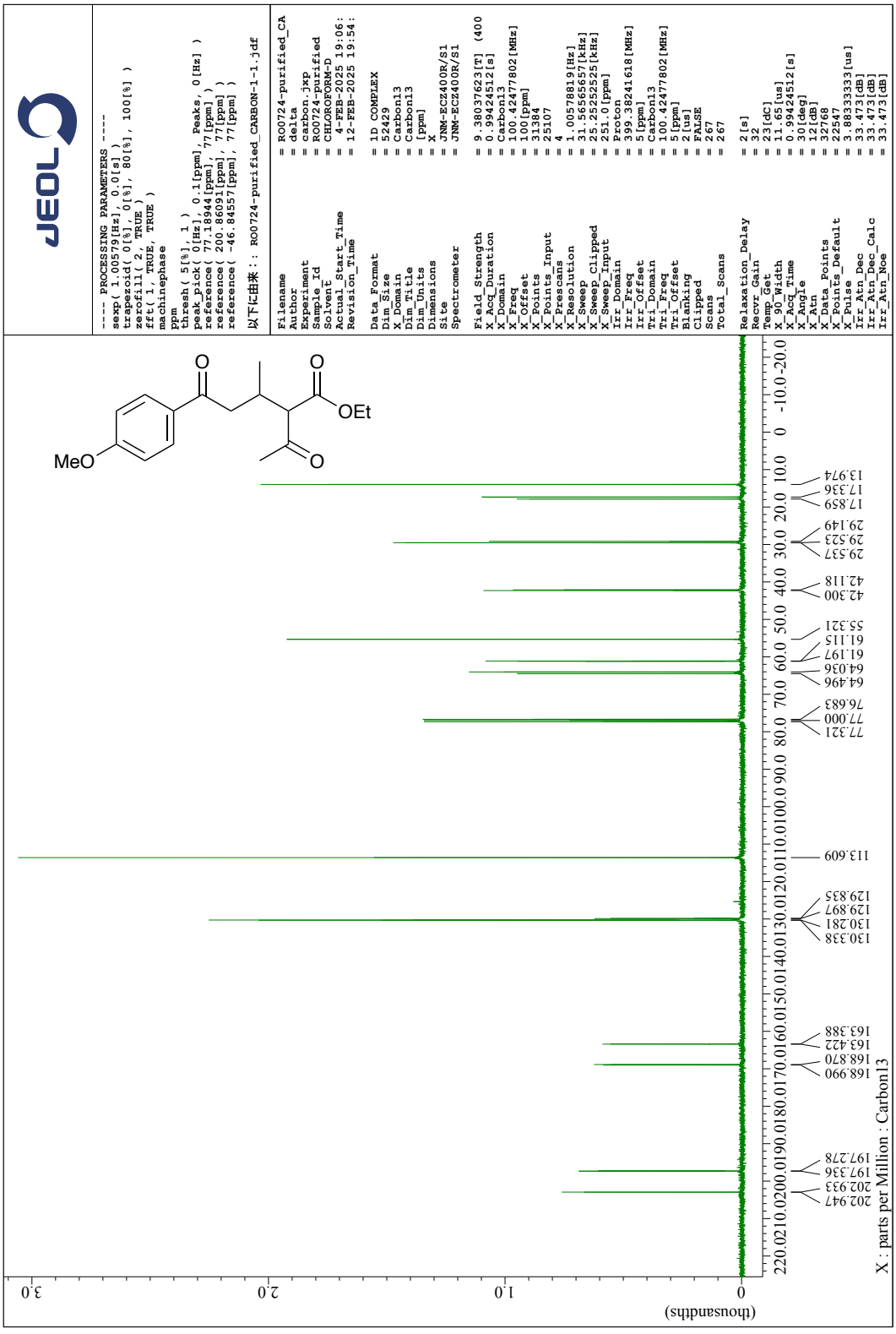

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.06435[ppm], 0[ppm])
thresh(5.43736[%], 1,)
Filename = RO0723-purified_PROT
Author = delta
Experiment = single_pulse.jxp
Sample_Id = RO0723-purified
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-FEB-2025 16:00:20
Revision_Time = 26-SEP-2025 10:33:13
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 32
Temp_Get = 21.9[dC]
X_90_Width = 8.87[us]
X_Acq_Time = 2.0487043[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
O
EtO
3.00
3.00
3.00
1.00
1.00
1.00
1.00
2.00
2.00
2.03
abundance
X : parts per Million : Proton
7.993
7.976
7.972
7.958
7.954
7.560
7.543
7.540
7.480
7.460
7.445
7.442
4.225
4.215
4.211
4.208
4.197
4.193
4.190
4.172
3.636
3.618
3.551
3.201
2.925
2.902
2.884
2.882
2.860
2.267
2.263
1.288
1.278
1.270
1.260
1.252
1.243
1.066
1.050
1.044
1.027

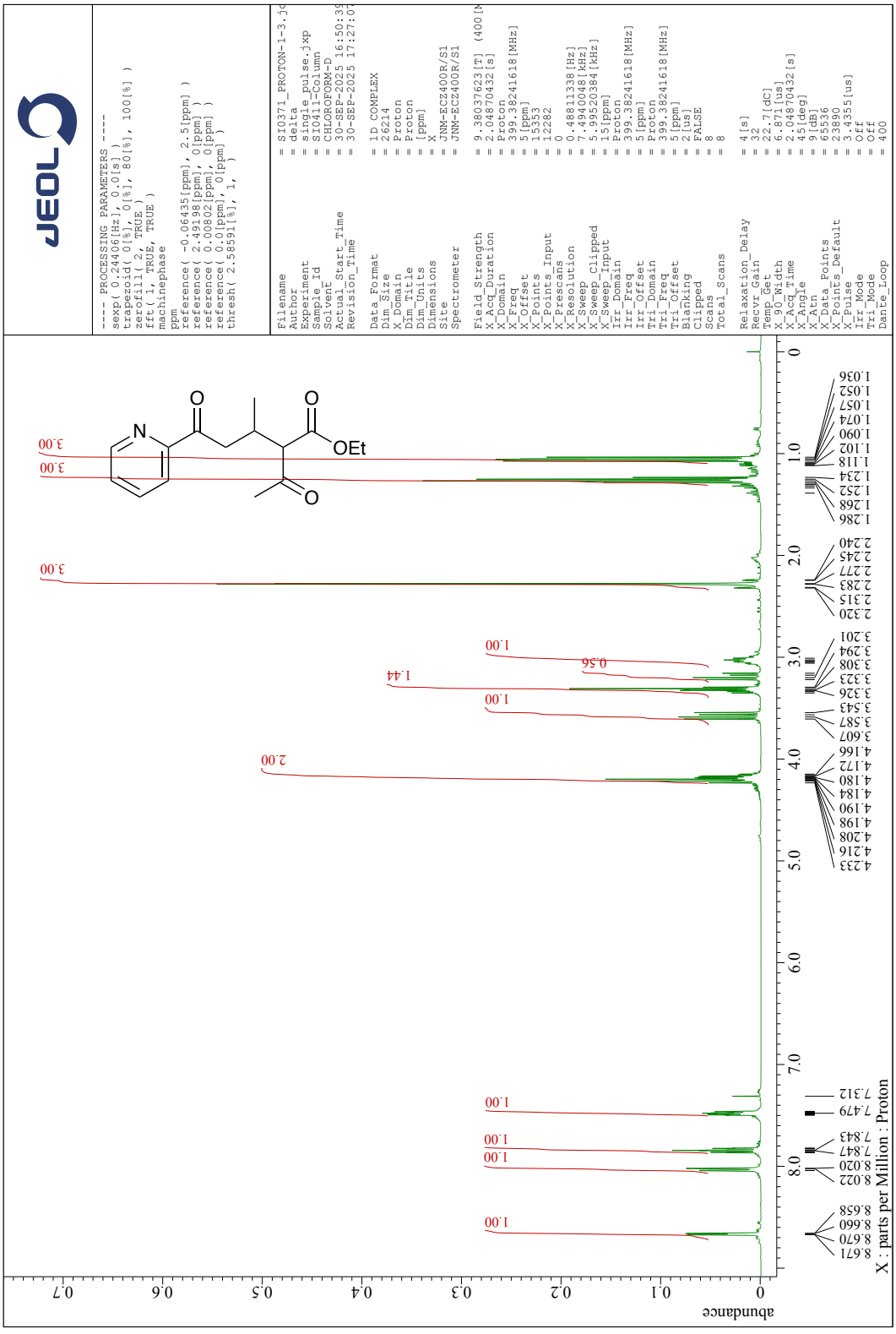
JEOL
---- PROCESSING PARAMETERS ----
expf(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.21822[ppm], 77[ppm])
以下に由来:: RO0723-purified_CARBON-1-1.jdf
Filename = RO0723-purified_CA
Author = delta
Experiment = carbon.jxp
Sample_Id = RO0723-purified
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-FEB-2025 16:01:
Revision_Time = 18-FEB-2025 14:36:
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 157
Total_Scans = 157
Relaxation_Delay = 2[s]
Recvr_Gain = 22
Temp_Get = 21.9[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Irr_Atn_Dec = 33.473[dB]
Irr_Atn_Dec_Calc = 33.473[dB]
Irr_Atn_Noe = 33.473[dB]
O
O
EtO
O
13.940
17.341
17.887
28.875
29.494
29.532
42.362
42.602
61.120
61.192
63.868
64.338
76.679
77.000
77.317
127.926
127.983
128.463
132.981
133.019
136.698
136.760
168.827
168.923
198.693
198.775
202.823
202.832
X : parts per Million : Carbon13
(thousandths)

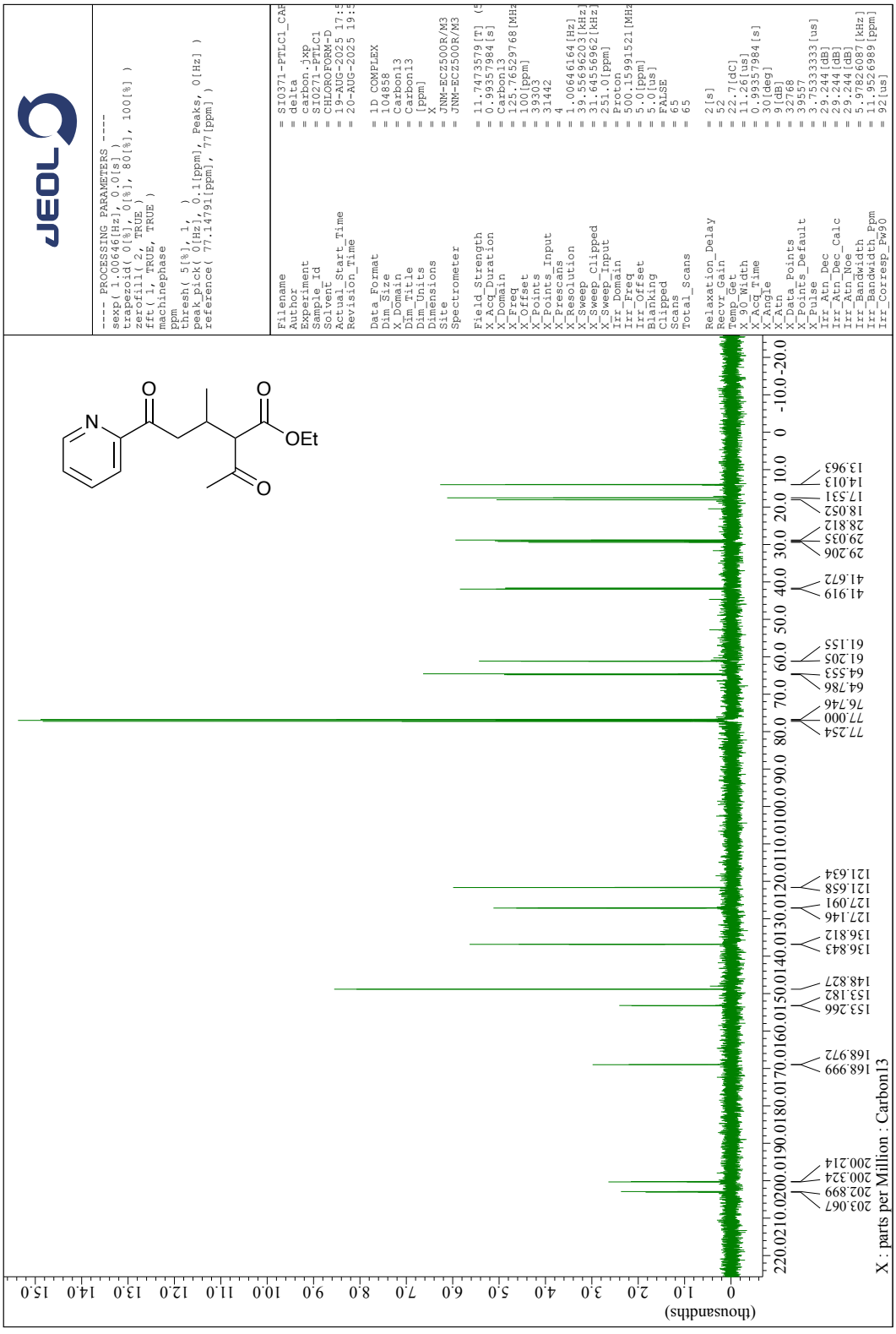

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.05118[ppm], 0[ppm])
thresh(3.52192[%], 1,)
Filename = RO0737-purified_PROT
Author = delta
Experiment = single_pulse.jxp
Sample_Id = RO0737-purified
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-FEB-2025 17:23:06
Revision_Time = 26-SEP-2025 11:22:51
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.1[dC]
X_90_Width = 8.8811[us]
X_Acq_Time = 2.0487[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
Me
EtO
O
O
O
3.00
3.00
3.00
2.00
2.00
2.00
1.00
1.00
1.00
1.00
7.894
7.875
7.855
7.298
7.267
7.247
4.227
4.223
4.213
4.209
4.205
4.195
4.192
4.188
4.170
3.627
3.609
3.558
3.539
3.160
3.149
3.107
2.891
2.865
2.404
2.265
2.260
1.279
1.271
1.261
1.243
1.057
1.040
1.033
1.016
X : parts per Million : Proton
abundance

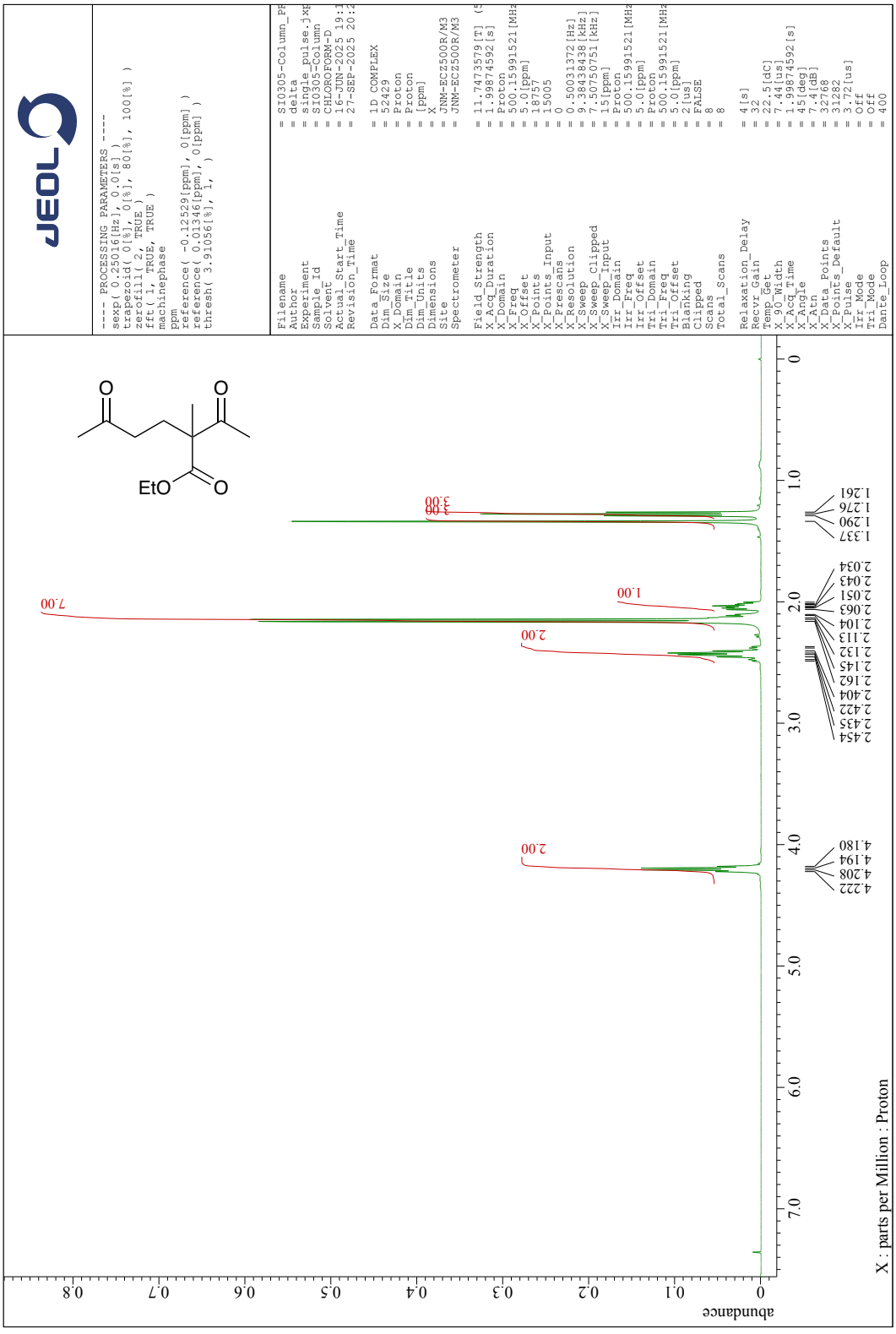

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.19424[ppm], 77[ppm])
以下に由来 : : RO0737-purified_CARBON-1-1.jdf
Filename = RO0737-purified_CARBON-1-1.jdf
Author = delta
Experiment = Carbon.jxp
Sample_Id = RO0737-purified
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-FEB-2025 17:24:32
Revision_Time = 26-SEP-2025 11:23:33
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 163
Total_Scans = 163
Relaxation_Delay = 2[s]
Recvr_Gain = 22
Temp_Get = 22.1[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Irr_Atn_Dec = 33.47[dB]
Irr_Atn_Dec_Calc = 33.47[dB]
Irr_Atn_Noe = 33.47[dB]
O
O
O
Me
EtO
O
(thousandths)
X : parts per Million : Carbon13
202.904
198.453
198.376
168.976
168.880
143.844
143.791
134.357
134.295
129.163
128.156
128.098
77.317
77.000
76.679
64.463
63.969
61.206
61.125
42.501
42.295
29.528
29.499
29.369
29.014
21.484
17.892
17.355
13.974

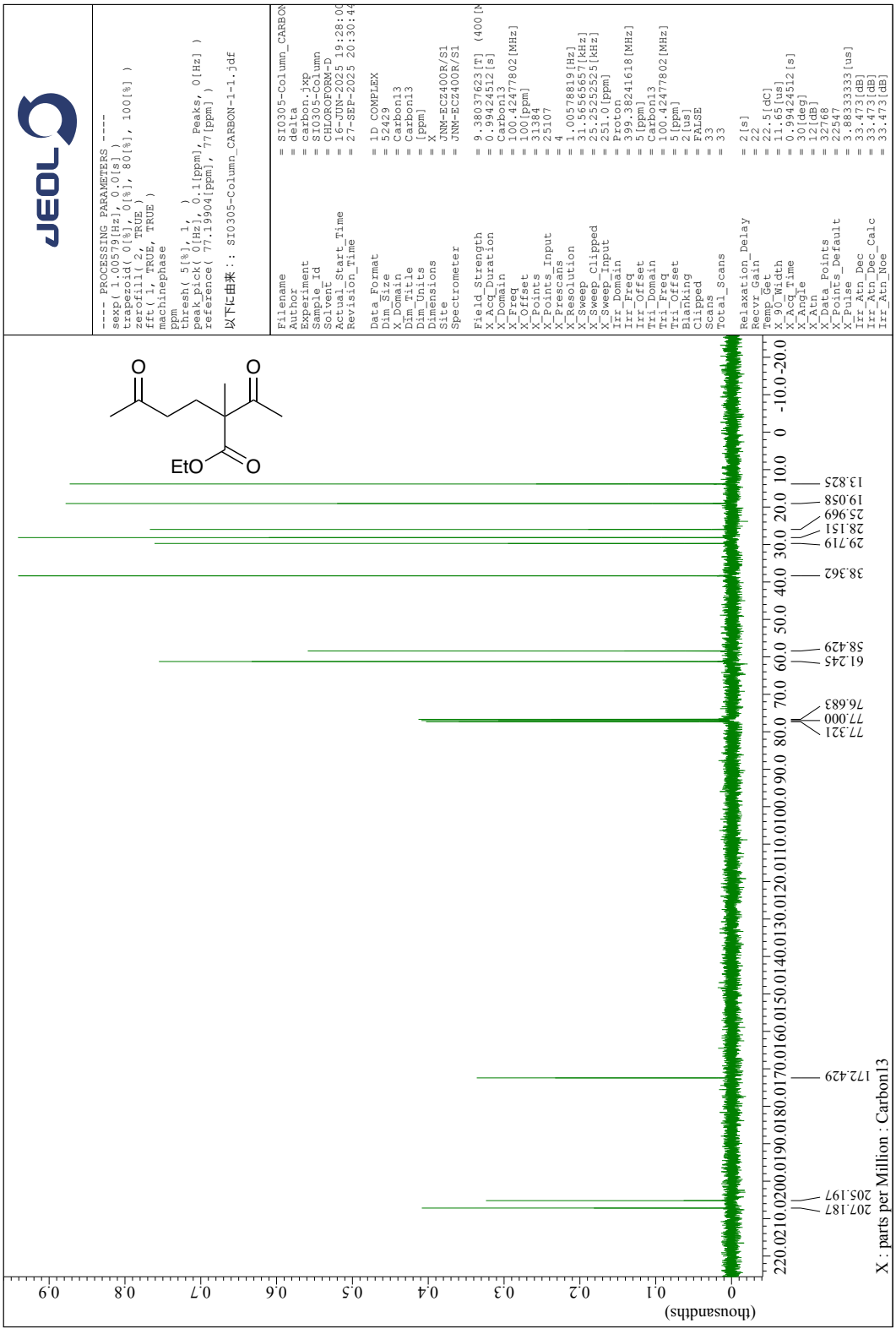

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.06321[ppm], 0[ppm])
thresh(2.4673[%], 1,)
Filename = RO0724-purified_PROT
Author = delta
Experiment = single_pulse.jxp
Sample_Id = RO0724-purified
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-FEB-2025 19:05:20
Revision_Time = 27-SEP-2025 15:57:41
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.9[dC]
X_90_Width = 8.8711[us]
X_Acq_Time = 2.04870432[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
MeO
OEt
O
O
O
3.00
3.00
3.00
2.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
7.986
7.982
7.965
7.944
6.954
6.947
6.925
6.919
4.225
4.214
4.207
4.196
4.189
4.178
4.171
3.902
3.865
3.625
3.606
3.138
3.084
2.845
2.822
2.804
2.782
2.267
2.262
1.281
1.274
1.263
1.245
1.054
1.036
1.031
1.014
abundance
X : parts per Million : Proton

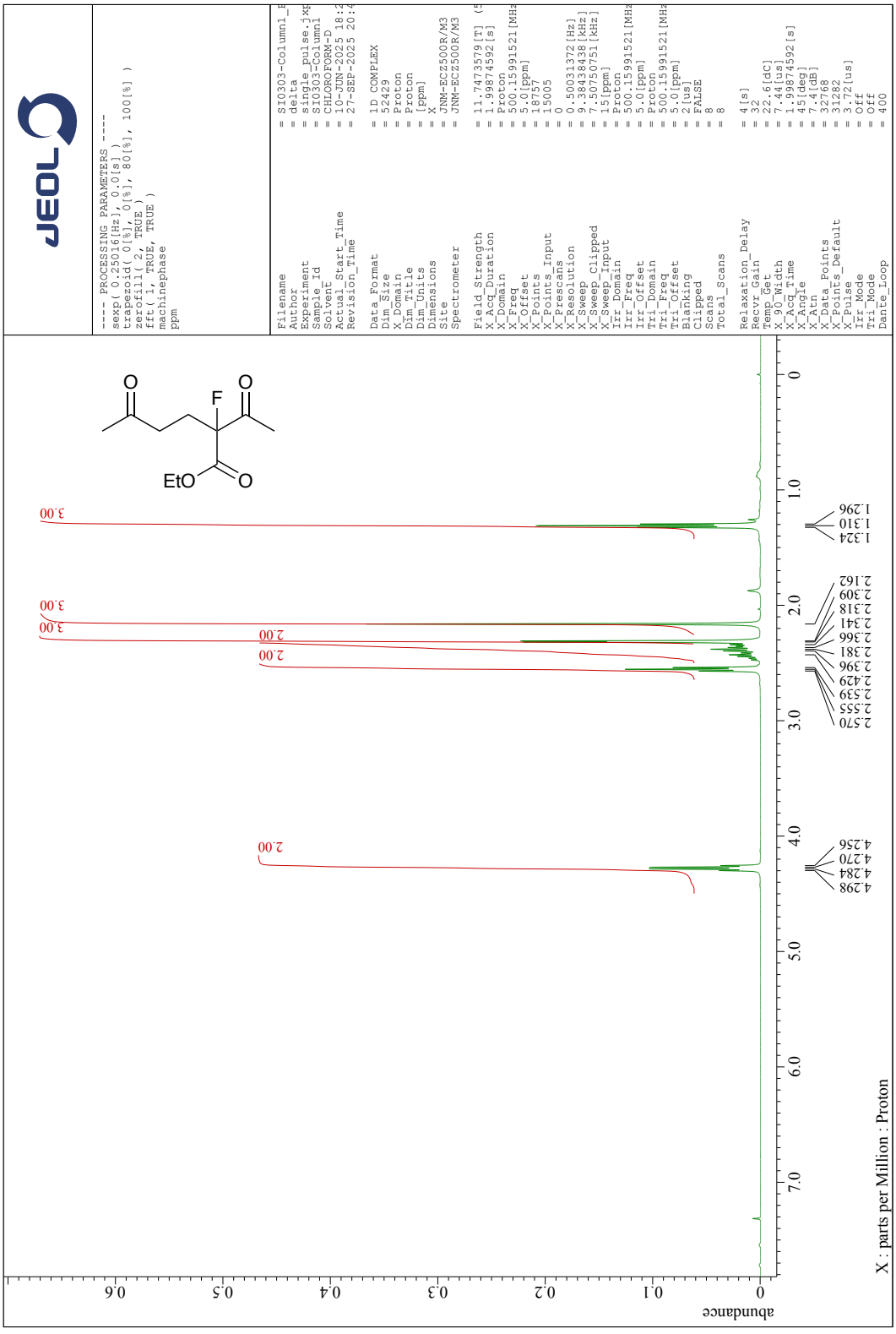

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.18944[ppm], 77[ppm])
reference(200.86091[ppm], 77[ppm])
reference(-46.84557[ppm], 77[ppm])
以下に由来：: RO0724-purified_CARBON-1-1.jdf
Filename = RO0724-purified_CA
Author = delta
Experiment = carbon.jxp
Sample_Id = RO0724-purified
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-FEB-2025 19:06:
Revision_Time = 12-FEB-2025 19:54:
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 267
Total_Scans = 267
Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Get = 23[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 0.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Irr_Atn_Dec = 33.473[dB]
Irr_Atn_Dec_Calc = 33.473[dB]
Irr_Atn_Noe = 33.473[dB]
MeO
O
O
OEt
O
(thousandths)
3.0
2.0
1.0
0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
202.947
202.933
197.336
197.278
168.990
168.870
163.422
163.388
130.338
130.281
129.897
129.835
113.609
77.321
77.000
76.683
64.496
64.036
61.197
61.115
55.321
42.300
42.118
29.537
29.523
29.149
17.859
17.336
13.974

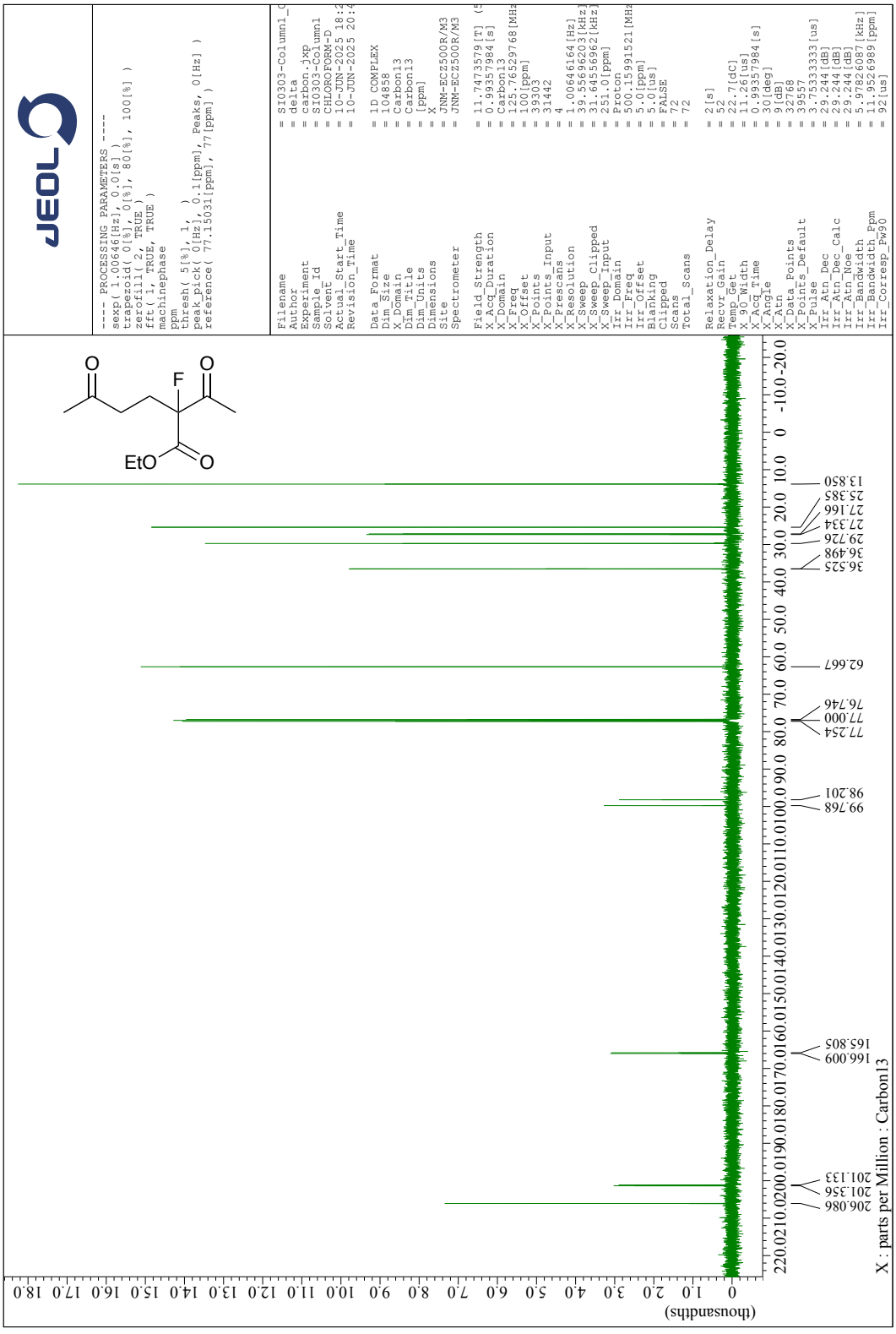

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.06435[ppm], 2.5[ppm])
reference(2.49198[ppm], 0[ppm])
reference(0.00802[ppm], 0[ppm])
reference(0.0[ppm], 0[ppm])
thresh(2.58591[%], 1,)
Filename = SI0371_PROTON-1-3.jd
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0411-Column
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-SEP-2025 16:50:39
Revision_Time = 30-SEP-2025 17:27:07
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.7[dC]
X_90_Width = 6.8711[us]
X_Acq_Width = 2.04870432[s]
X_Acq_Time = 2.0487[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
N
O
O
O
OEt
3.00
3.00
3.00
2.00
1.00
1.44
1.00
0.56
1.00
1.00
1.00
1.00
8.671
8.670
8.660
8.658
8.022
8.020
7.847
7.843
7.479
7.312
4.233
4.216
4.208
4.198
4.190
4.184
4.180
4.172
4.166
3.607
3.587
3.543
3.326
3.323
3.308
3.294
3.201
2.320
2.315
2.283
2.277
2.245
2.240
1.286
1.268
1.252
1.234
1.118
1.102
1.090
1.074
1.057
1.052
1.036
X : parts per Million : Proton
abundance

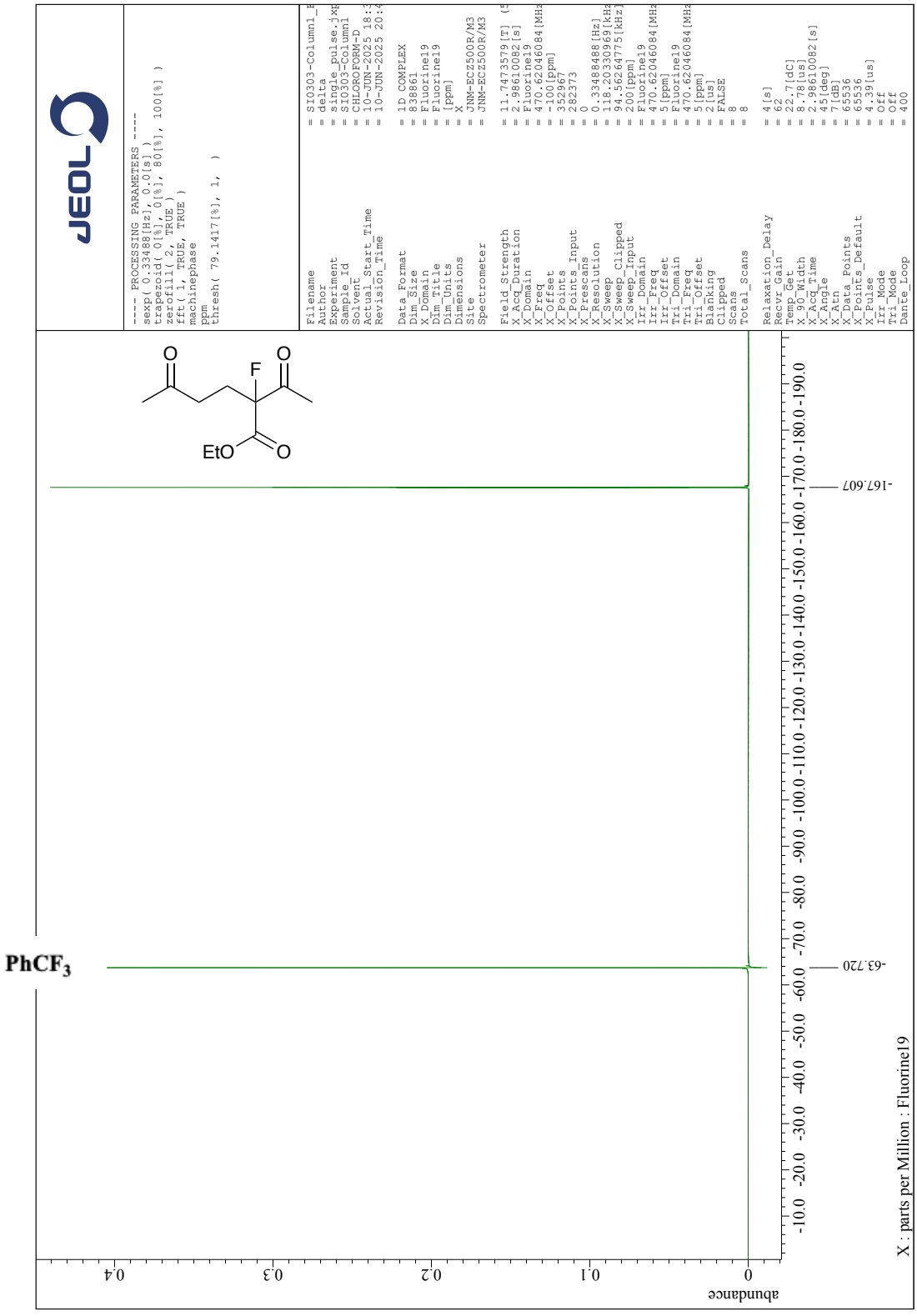

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00646[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.14791[ppm], 77[ppm])
Filename = S10371-PTLC1_CAF
Author = delta
Experiment = carbon.jxp
SampleId = S10271-PTLC1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-AUG-2025 17:5
Revision_Time = 20-AUG-2025 19:5
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Carbon13
DIm_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.74735579[T] (5
X_Acq_Duration = 0.99357984[s]
X_Domain = Carbon13
X_Freq = 125.765297.68[MHz
X_Offset = 100[ppm]
X_Points = 39303
X_Points_Input = 31442
X_Prescans = 4
X_Resolution = 1.00646164[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 65
Total_Scans = 65
Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Get = 22.7[dC]
X_90_Width = 11.26[us]
X_Acq_Time = 0.99357984[s]
X_Angle = 90[deg]
X_Atn = 3[dB]
X_Data_Points = 39557
X_Pulse_Default = 3.75333333[us]
Irr_Atn_Dec = 29.244[dB]
Irr_Atn_Dec_Calc = 29.244[dB]
Irr_Atn_Noe = 29.244[dB]
Irr_Bandwidth = 5.97826087[kHz]
Irr_Bandwidth_Ppm = 11.9526989[ppm]
Irr_Corresp_Pw90 = 92[us]
N
O
O
O
OEt
203.067
202.899
200.324
200.214
168.999
168.972
153.266
153.182
148.827
136.843
136.812
127.146
127.091
121.658
121.634
77.254
77.000
76.746
64.786
64.553
61.205
61.155
41.672
41.919
29.206
29.035
28.812
18.052
17.531
14.013
13.963
(thousandths)
X : parts per Million : Carbon13

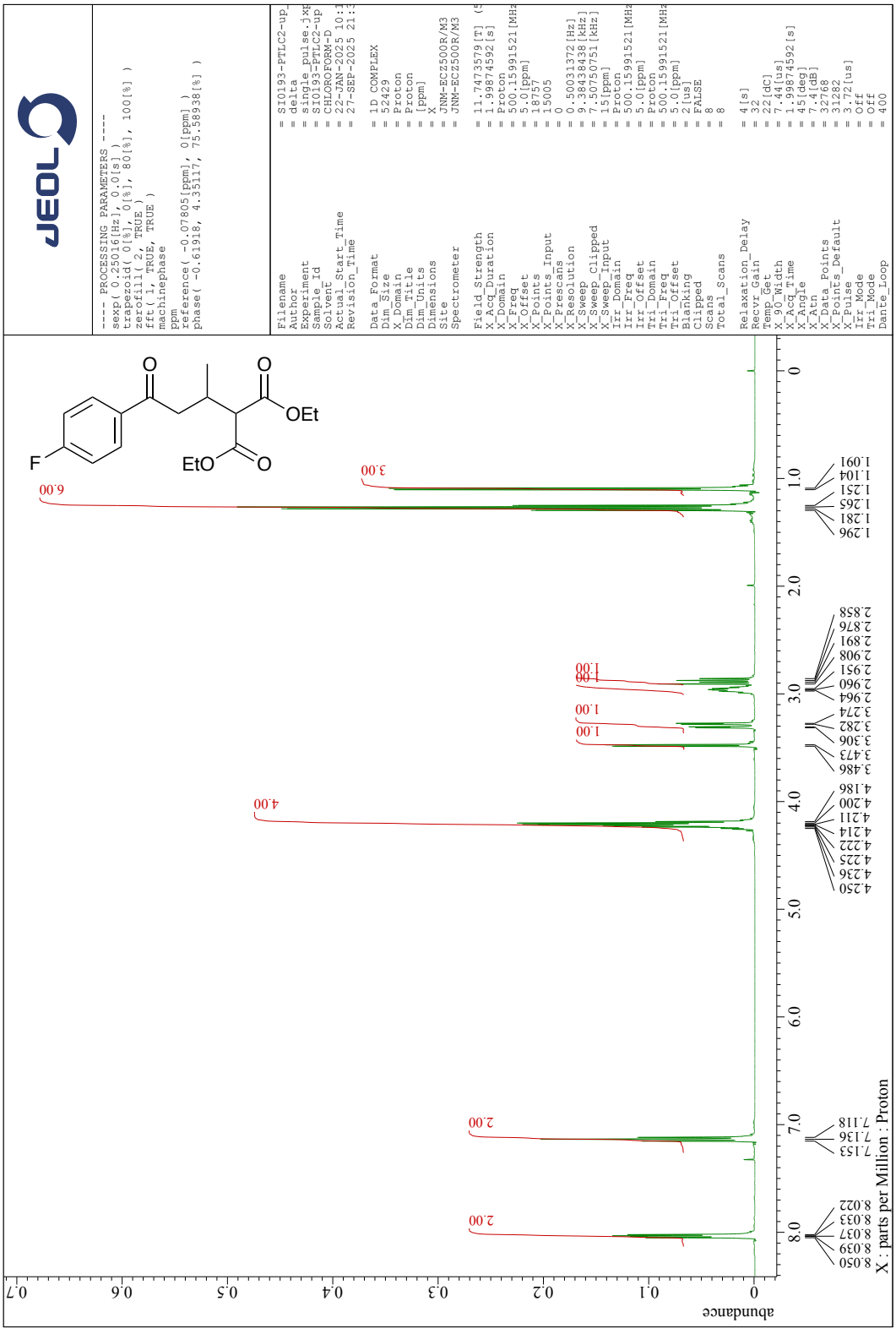

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.25016[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.12529[ppm], 0[ppm])
reference(0.01346[ppm], 0[ppm])
thresh(3.91056[%], 1,)
Filename = SI0305-Column_PF
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0305-Column
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-JUN-2025 19:1
Revision_Time = 27-SEP-2025 20:4
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.7473579[T]
X_Acq_Duration = 1.99874592[s]
X_Domain = Proton
X_Freq = 500.15991521[MHz
X_Offset = 5.0[ppm]
X_Points = 18757
X_Points_Input = 15005
X_Prescans = 0
X_Resolution = 0.50031372[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz
Tri_Offset = 5.0[ppm]
Blanking = 21[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 32
Temp_Get = 22.5[dC]
X_90_Width = 7.40[us]
X_Acq_Time = 1.99874592[s]
X_Angle = 45[deg]
X_Atn = 7.4[dB]
X_Data_Points = 32768
X_Points_Default = 31282
X_Pulse = 3.72[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
O
EtO
7.00
1.00
2.00
2.00
3.00
3.00
1.337
1.290
1.276
1.261
2.454
2.435
2.422
2.404
2.162
2.145
2.132
2.113
2.104
2.063
2.051
2.043
2.034
4.222
4.208
4.194
4.180
abundance
X : parts per Million : Proton

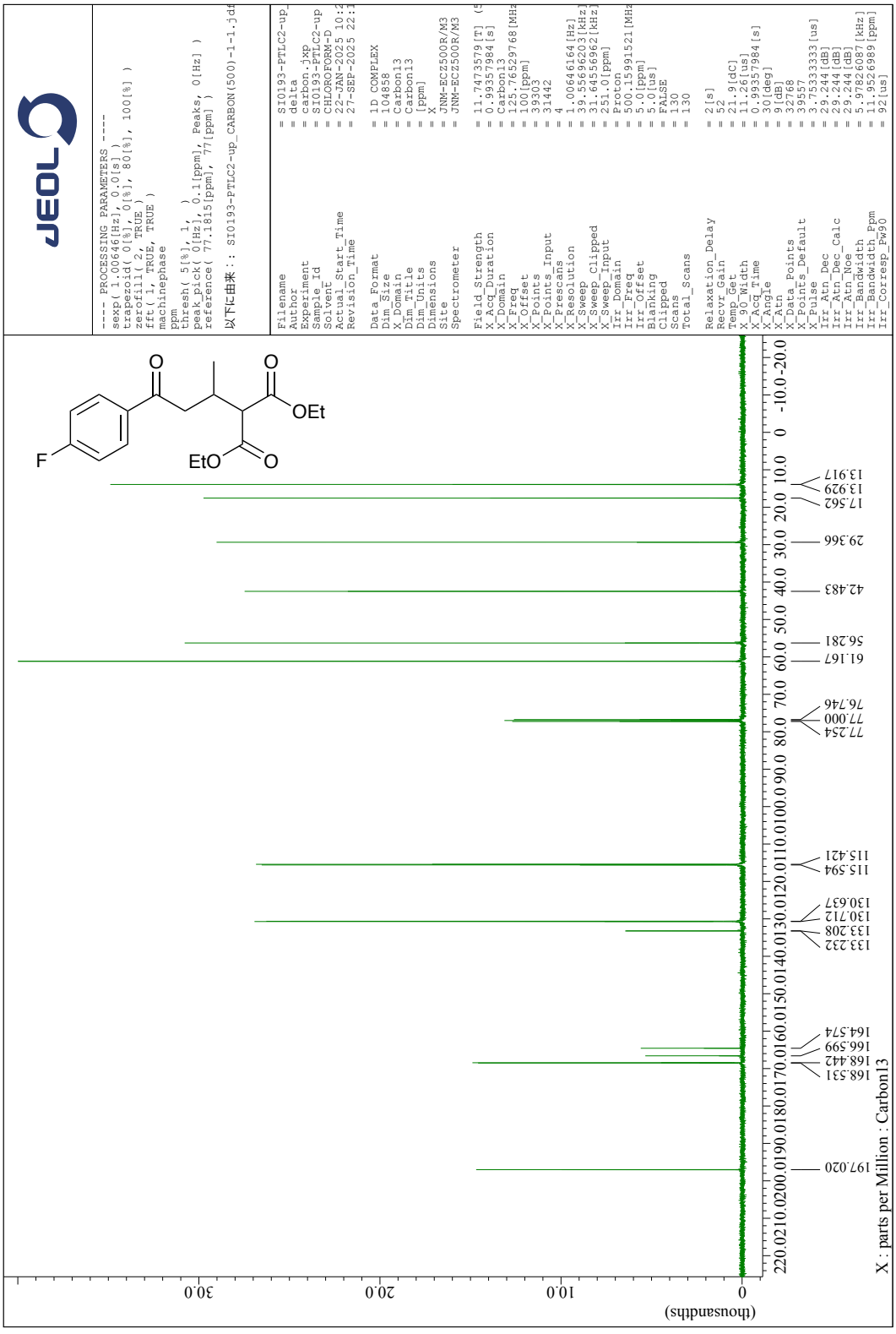

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.19904[ppm], 77[ppm])
以下に由来 : : SI0305-Column_CARBON-1-1.jdf
Filename = SI0305-Column_CARBON
Author = delta
Experiment = Carbon.jxp
Sample_Id = SI0305-Column
SolventE = CHLOROFORM-D
Actual_Start_Time = 16-JUN-2025 19:28:00
Revision_Time = 27-SEP-2025 20:30:44
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 33
Total_Scans = 33
Relaxation_Delay = 2[s]
Recvr_Gain = 22
Temp_Get = 22.5[dC]
X_90_Width = 11.65[us]
X_Acq_Time = 1.99424512[s]
X_Atn = 3[dB]
X_Atn_Dec = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Ir_Atn_Dec = 33.47[dB]
Ir_Atn_Dec_Calc = 33.47[dB]
Irr_Atn_Noe = 33.47[dB]
O
O
O
EtO
(thousandths)
X : parts per Million : Carbon13
207.187
205.197
172.429
77.321
77.000
76.683
61.245
58.429
38.362
29.719
28.151
25.969
19.058
13.825


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.25016[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = ST0303-Column1_E
Author = delta
Experiment = single_pulse_1H
SampleId = ST0303-Column1
SolvenT = CHLOROFORM-D
Actual_Start_Time = 10-JUN-2025 18:2
Revision_Time = 27-SEP-2025 20:4
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Proton
DIm_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.7473579[T]
X_Acq_Duration = 1.998745 92[s]
X_Domain = Proton
X_Freq = 500.15991521[MHz
X_Offset = 5.0[ppm]
X_Points = 18757
X_Points_Input = 15005
X_Prescans = 0
X_Resolution = 0.50031372[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz
Tri_Offset = 5.0[ppm]
Blanking = 21us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 32
Temp_Get = 22.6[dC]
X_90_Width = 7.49[us]
X_Acq_Time = 1.998745 92[s]
X_Angle = 45[deg]
X_Atn = 7.4[dB]
X_Data_Points = 32768
X_Points_Default = 31282
X_Pulse = 3.72[us]
Irr_Mode = Off
Tri_Mode = Off
Date_Loop = 400
O
F
O
EtO
O
3.00
3.00
3.00
2.00
2.00
2.00
1.324
1.310
1.296
2.570
2.555
2.539
2.429
2.396
2.381
2.366
2.341
2.318
2.309
2.162
4.298
4.284
4.270
4.256
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
X : parts per Million : Proton

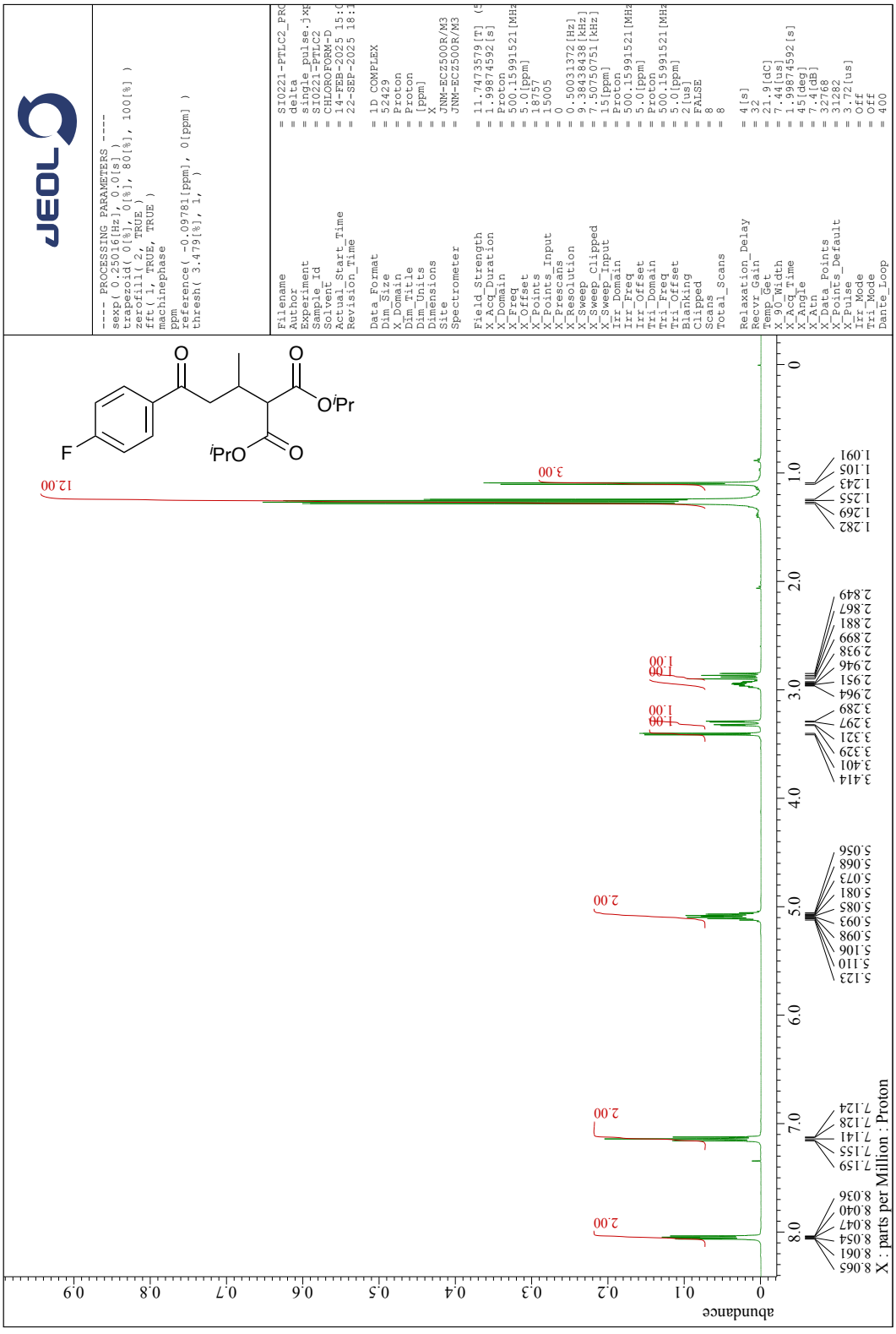

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00646[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.15031[ppm], 77[ppm])
Filename = ST0303-Column1_C
Author = delta
Experiment = carbon.jxp
SampleId = ST0303-Column1
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-JUN-2025 18:2
Revision_Time = 10-JUN-2025 20:4
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ500R/M3
Spectrometer = JNM-ECZ500R/M3
Field_Strength = 11.7473579[T] (5
X_Acq_Duration = 0.99357984[s]
X_Domain = Carbon13
X_Freq = 125.765297.68[MHz
X_Offset = 100[ppm]
X_Points = 39303
X_Points_Input = 31442
X_Prescans = 4
X_Resolution = 1.00646164[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 72
Total_Scans = 72
Relaxation_Delay = 2[s]
Recvr_Gain = 52
Temp_Get = 22.7[dC]
X_90_Width = 11.26[us]
X_Acq_Time = 0.99357984[s]
X_Angle = 90[deg]
X_Atn = 32[dB]
X_Data_Points = 39557
X_Points_Default = 3.75333333[us]
Irr_Atn_Dec = 29.244[dB]
Irr_Atn_Dec_Calc = 29.244[dB]
Irr_Atn_Noe = 29.244[dB]
Irr_Bandwidth = 5.97826087[kHz]
Irr_Bandwidth_Ppm = 11.9526989[ppm]
Irr_Corresp_Pw90 = 92[us]
O
F
O
EtO
O
13.850
25.385
27.166
27.334
29.726
36.498
36.525
62.667
76.746
77.000
77.254
98.201
99.768
165.805
166.009
201.133
201.356
206.086
(thousandths)
X : parts per Million : Carbon13

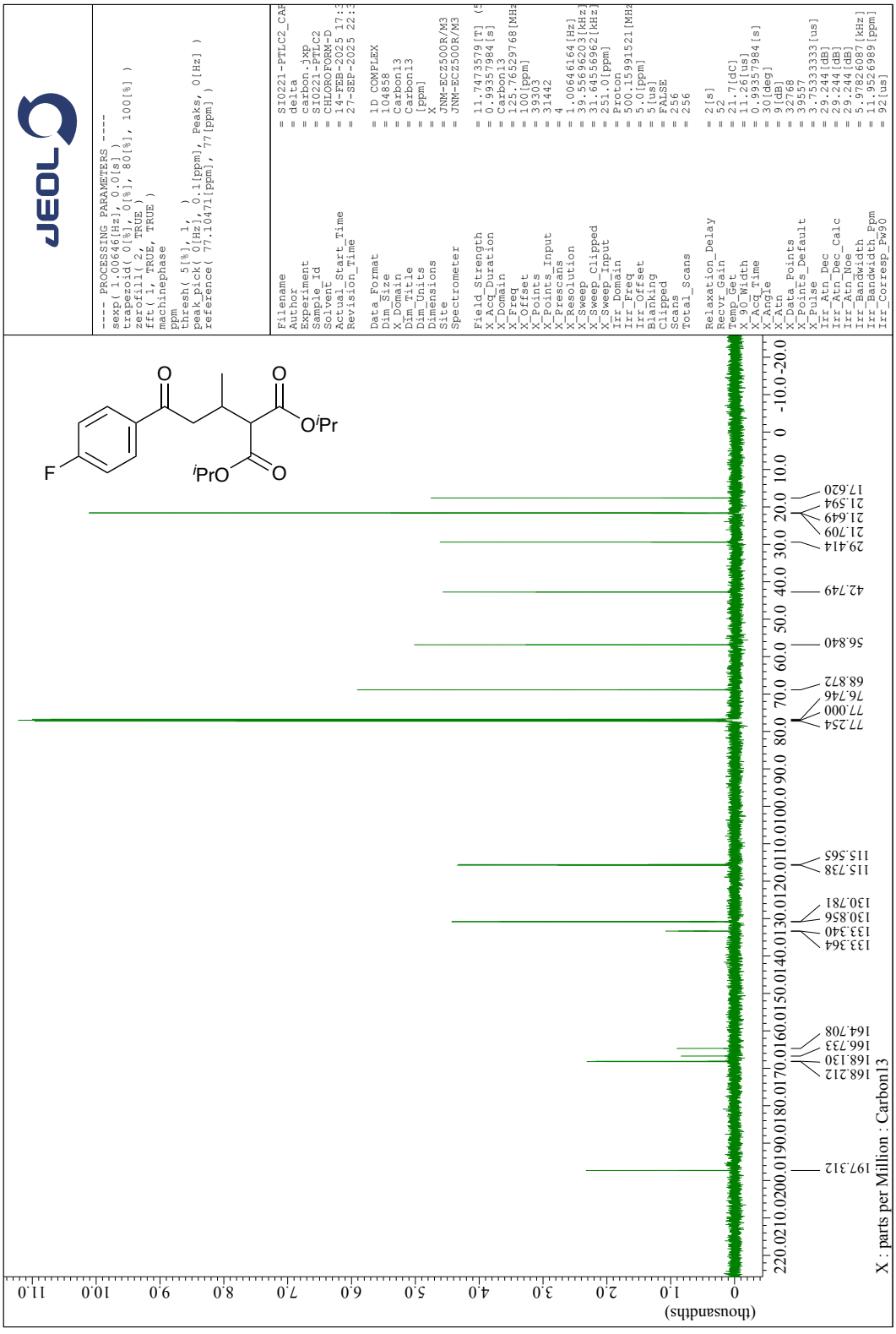

PhCF3
-63.720
-167.607
X : parts per Million : Fluorine19
abundance
F
O
O
EtO
O


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.25016[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.07805[ppm], 0[ppm])
phase(-0.61918, 4.35117, 75.58938[%])
Filename = ST0193-PTLC2-up_
Author = delta
Experiment = single_pulse_1H
SampleId = ST0193-PTLC2-up
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JAN-2025 10:1
Revision_Time = 27-SEP-2025 21:3
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.7473579[T]
X_Acq_Duration = 1.99874592[s]
X_Domain = Proton
X_Freq = 500.15991521[MHz
X_Offset = 5.0[ppm]
X_Points = 18757
X_Points_Input = 15005
X_Prescans = 0
X_Resolution = 0.50031372[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz
Tri_Offset = 5.0[ppm]
Blanking = 21[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 32
Temp_Get = 22[dC]
X_90_Width = 7.44[us]
X_Acq_Time = 1.99874592[s]
X_Angle = 45[deg]
X_Atn = 7.4[dB]
X_Data_Points = 32768
X_Points_Default = 31282
X_Pulse = 3.72[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
OEt
F
EtO
O
6.00
3.00
4.00
2.00
2.00
1.00
1.00
1.00
2.00
abundance
X : parts per Million : Proton

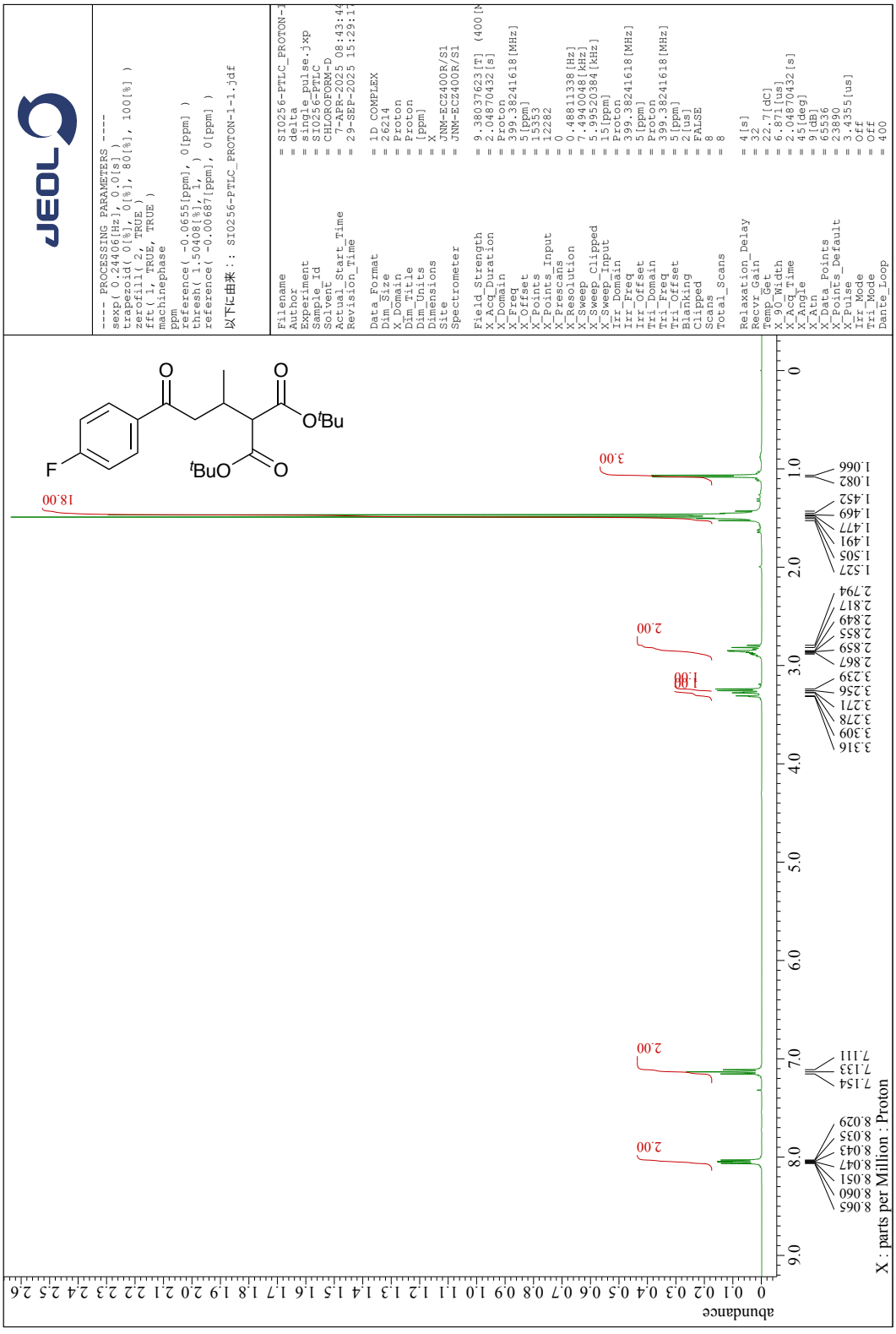

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00646[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.1815[ppm], 77[ppm])
以下に由来：: SI0193-PTLC2-up_CARBON(500)-1-1.jdf
Filename = SI0193-PTLC2-up_
Author = delta
Experiment = carbon.jxp
Sample_Id = SI0193-PTLC2-up
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JAN-2025 10:2
Revision_Time = 27-SEP-2025 22:1
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.74735579[T] (5
X_Acq_Duration = 0.99357984[s]
X_Domain = Carbon13
X_Freq = 125.765297.68[MHz
X_Offset = 100[ppm]
X_Points = 39303
X_Points_Input = 31442
X_Prescans = 4
X_Resolution = 1.00646164[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 130
Total_Scans = 130
Relaxation_Delay = 2[s]
Recvr_Gain = 52
Temp_Get = 21.9[dC]
X_90_Width = 11.26[us]
X_Acq_Time = 0.99357984[s]
X_Angle = 90[deg]
X_Atn = 32[dB]
X_Data_Points = 39557
X_Points_Default = 3.75333333[us]
Irr_Atn_Dec = 29.244[dB]
Irr_Atn_Dec_Calc = 29.244[dB]
Irr_Atn_Noe = 29.244[dB]
Irr_Bandwidth = 5.97826087[kHz]
Irr_Bandwidth_Ppm = 11.9526989[ppm]
Irr_Corresp_Pw90 = 92[us]
F
O
O
OEt
EtO
O
168.531
168.442
166.599
164.574
197.020
115.594
115.421
133.232
133.208
130.712
130.637
77.254
77.000
76.746
61.167
56.281
42.483
29.366
17.562
13.929
13.917
(thousandths)
X : parts per Million : Carbon13

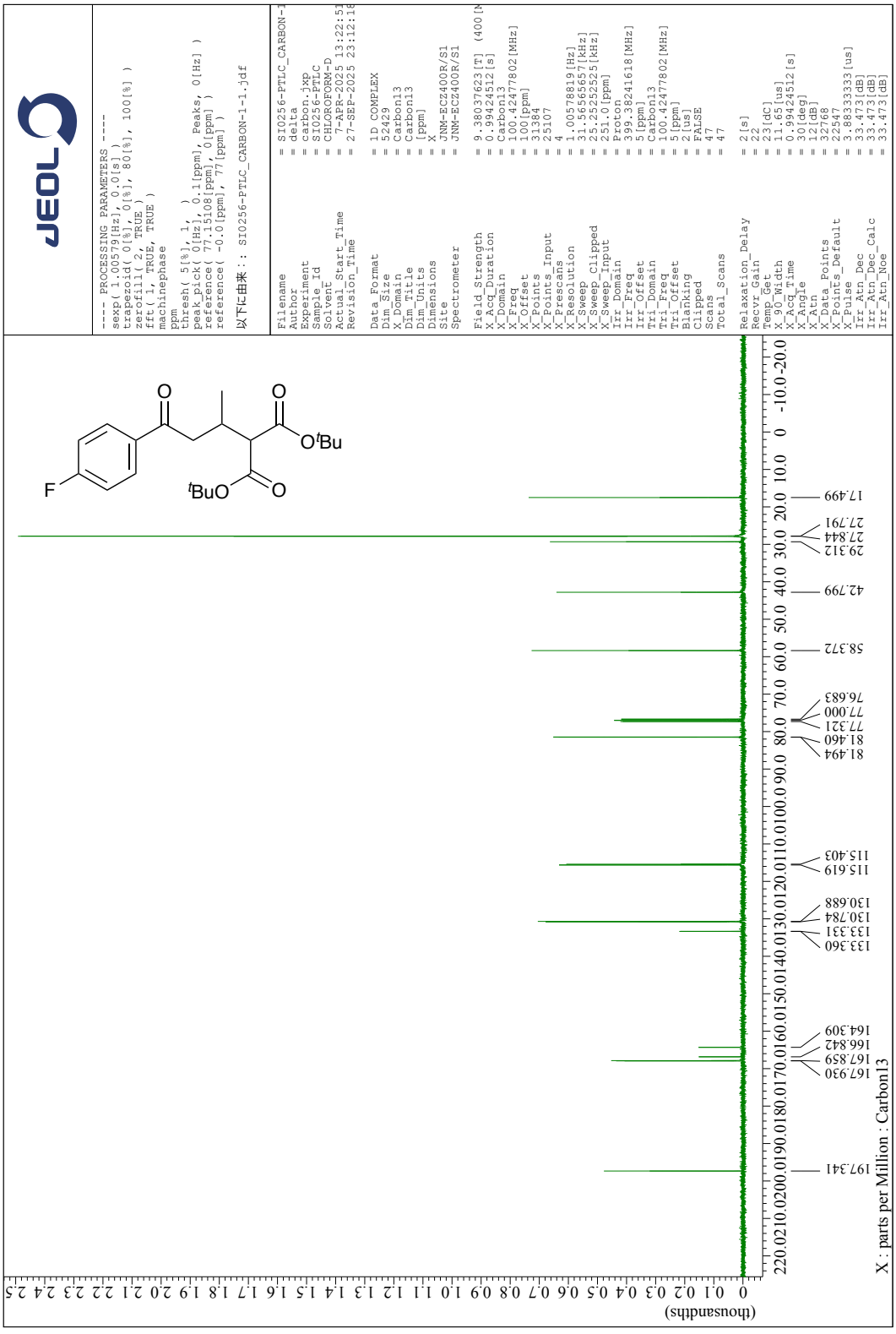
JEOL
---- PROCESSING PARAMETERS ----
sexp(0.33488[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.70814[ppm], 0[ppm])
reference(0.14301[ppm], -63.72[ppm])
reference(-176.04218[ppm], -63.72[ppm])
thresh(4.65489[%], 0.04658[%], 0.02182[abn])
reference(48.46938[ppm], -63.72[ppm])
Filename = ST0193-PTLC2-up_
Author = delta
Experiment = single_pulse_dx
Sample_Id = ST0193-PTLC2-up
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JAN-2025 12:4
Revision_Time = 27-SEP-2025 22:1
Data_Format = 1D COMPLEX
Dim_Size = 838861
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.7473579[T] (5
X_Acq_Duration = 2.98610082[s]
X_Domain = Fluorine19
X_Freq = 470.62046084[MHz
X_Offset = -100[ppm]
X_Points = 352967
X_Points_Input = 282373
X_Prescans = 0
X_Resolution = 0.33488488[Hz]
X_Sweep = 118.20330969[kHz
X_Sweep_Clipped = 94.56264775[kHz]
X_Sweep_Input = 200[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 470.62046084[MHz
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 470.62046084[MHz
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 52
Temp_Get = 22.1[dC]
X_90_Width = 5.78[us]
X_Acq_Time = 2.98610082[s]
X_Angle = 45[deg]
X_Atn = 7[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.39[us]
Ir_Mode = Off
Tri_Mode = Off
Date_Loop = 400
O
O
OEt
F
EtO
O
PhCF3
-106.335
abundance
0
0.1
0.2
0.3
0.4
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
X : parts per Million : Fluorine19


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.25016[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.09781[ppm], 0[ppm])
thresh(3.479[%], 1,)
Filename = S10221-PTLC2_PRO
Author = delta
Experiment = single_pulse.jxp
Sample_Id = S10221-PTLC2
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-FEB-2025 15:0
Revision_Time = 22-SEP-2025 18:1
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.74735791[T] (5
X_Acq_Duration = 1.99874592[s]
X_Domain = Proton
X_Freq = 500.15991521[MHz
X_Offset = 5.0[ppm]
X_Points = 18757
X_Points_Input = 15005
X_Prescans = 0
X_Resolution = 0.50031372[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz
Tri_Offset = 5.0[ppm]
Blanking = 21[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 32
Temp_Get = 21.9[dC]
X_90_Width = 7.45[us]
X_Acq_Time = 1.99874592[s]
X_Angle = 45[deg]
X_Atn = 7.4[dB]
X_Data_Points = 32768
X_Points_Default = 31282
X_Pulse = 3.72[us]
Irr_Mode = Off
Tri_Mode = Off
Date_Loop = 400
O
O
O
O
iPr
iPrO
F
12.00
3.00
2.00
2.00
2.00
1.00
1.00
1.00
8.065
8.061
8.054
8.047
8.040
8.036
7.159
7.155
7.141
7.128
7.124
5.123
5.110
5.106
5.098
5.093
5.085
5.081
5.073
5.068
5.056
3.414
3.401
3.329
3.321
3.297
3.289
2.964
2.951
2.946
2.938
2.899
2.881
2.867
2.849
1.282
1.269
1.255
1.243
1.105
1.091
abundance
X : parts per Million : Proton

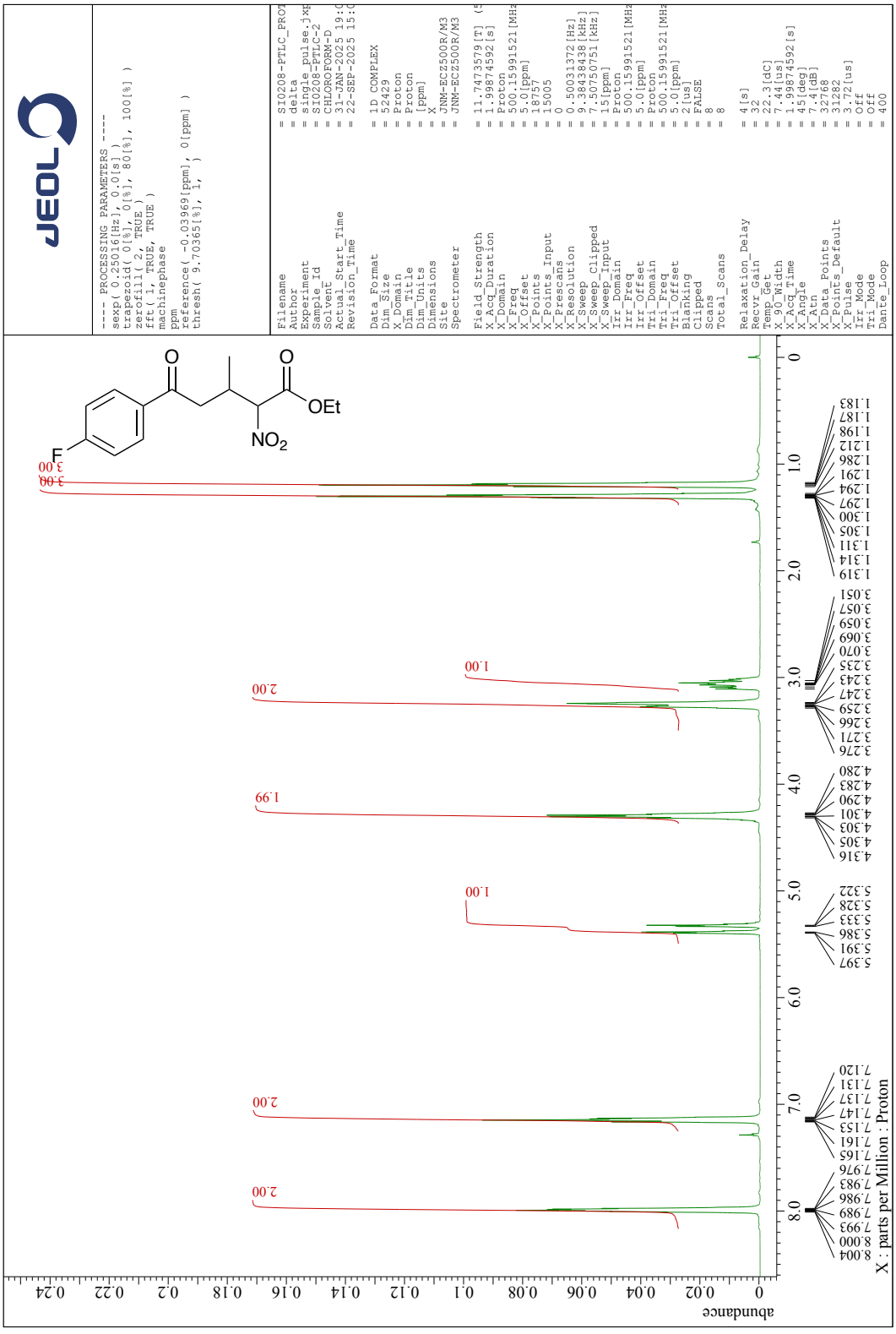

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00646[Hz], 0.01[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.10471[ppm], 77[ppm])
Filename = S10221-PTLC2_CAR
Author = delta
Experiment = carbon.jxp
SampleId = S10221-PTLC2
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-FEB-2025 17:3
Revision_Time = 27-SEP-2025 22:3
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.74735579[T] (5
X_Acq_Duration = 0.99357984[s]
X_Domain = Carbon13
X_Freq = 125.765297.68[MHz
X_Offset = 100[ppm]
X_Points = 39303
X_Points_Input = 31442
X_Prescans = 4
X_Resolution = 1.00646164[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 52
Temp_Get = 21.7[dC]
X_90_Width = 11.26[us]
X_Acq_Time = 0.99357984[s]
X_Angle = 90[deg]
X_Atn = 32[dB]
X_Data_Points = 39557
X_Points_Default = 3.75333333[us]
Irr_Atn_Dec = 29.244[dB]
Irr_Atn_Dec_Calc = 29.244[dB]
Irr_Atn_Noe = 29.244[dB]
Irr_Bandwidth = 5.97826087[kHz]
Irr_Bandwidth_Ppm = 11.95269891[ppm]
Irr_Corresp_Pw90 = 92[us]
O
O
O
O
F
iPrO
O
iPr
(thousandths)
X : parts per Million : Carbon13
197.312
168.212
168.130
166.733
164.708
133.364
133.340
130.856
130.781
115.738
115.565
77.254
77.000
76.746
68.872
56.840
42.749
29.414
21.709
21.649
21.594
17.620

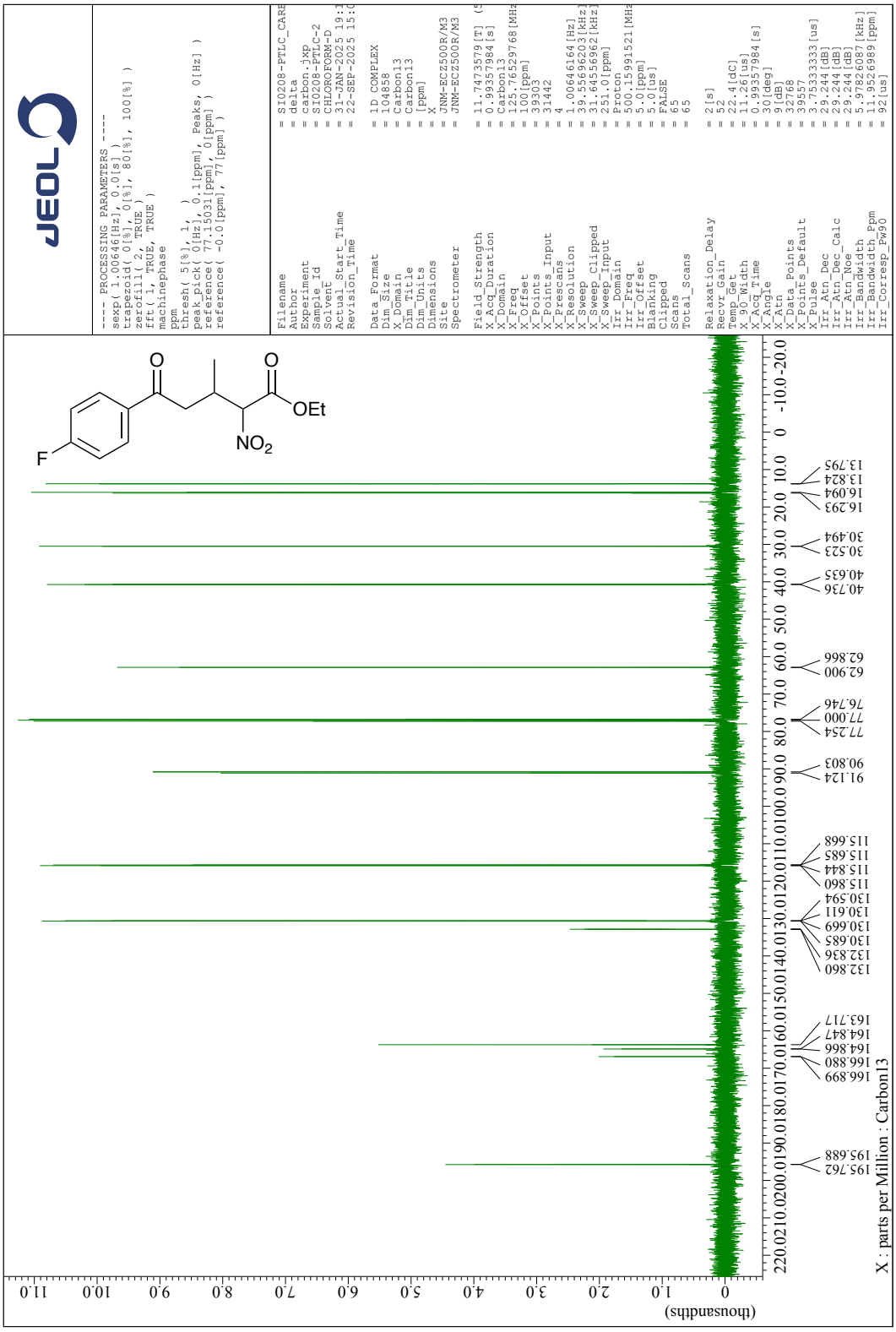
JEOL
---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.27833[ppm], -63.72[ppm])
reference(-102.3702[ppm], -63.72[ppm])
reference(-25.68691[ppm], -63.72[ppm])
reference(-63.41191[ppm], -63.72[ppm])
thresh(84.2563[%], 1,)
reference(-63.7325[ppm], -63.72[ppm])
reference(-63.59888[ppm], -63.72[ppm])
Filename = SI0221-PTLC2_Fluorir
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0221-PTLC2
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-FEB-2025 20:39:09
Revision_Time = 30-AUG-2025 10:10:44
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.0338032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.7[dC]
X_90_Width = 2.5[us]
X_Acq_Time = 2.0338032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Ir_Mode = Off
Tri_Mode = Off
Date_Loop = 400
O
O
O
O/iPr
F
iPrO
PhCF3
-106.349
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-190.0
X : parts per Million : Fluorine19


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.0655[ppm], 0[ppm])
thresh(1.50408[%], 1,)
reference(-0.00687[ppm], 0[ppm])
以下に由来：: SI0256-PTLC_PROTON-1-1.jdf
Filename = SI0256-PTLC_PROTON-1
Author = delta
Experiment = Single_pulse.jxp
Sample_Id = SI0256-PTLC
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-APR-2025 08:43:44
Revision_Time = 29-SEP-2025 15:29:1
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22.7[dC]
Temp_Get = 21.8[deg]
X_90_Width = 2.0487[us]
X_Acq_Time = 2.04870432[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
O
O
F
tBuO
O
18.00
3.00
2.00
2.00
1.00
2.00
8.065
8.060
8.051
8.047
8.043
8.035
8.029
7.154
7.133
7.111
3.316
3.309
3.278
3.271
3.256
3.239
2.867
2.859
2.855
2.849
2.817
2.794
1.527
1.505
1.491
1.477
1.469
1.452
1.082
1.066
abundance
X : parts per Million : Proton

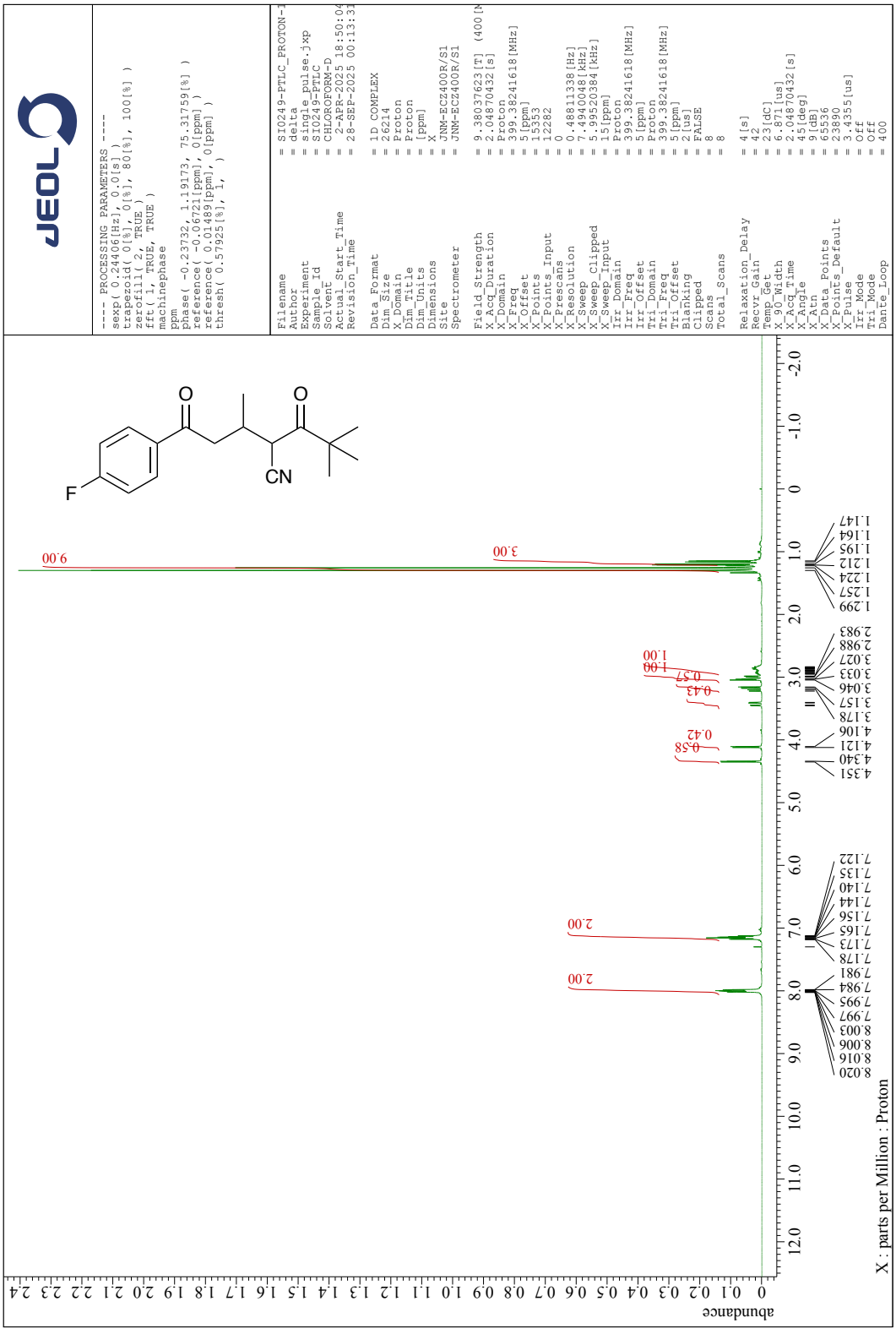

JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.15108[ppm], 0[ppm])
reference(-0.0[ppm], 77[ppm])
以下に由来 : : SI0256-PTLC_CARBON-1-1.jdf
Filename = SI0256-PTLC_CARBON-1
Author = delta
Experiment = Carbon.jxp
Sample_Id = SI0256-PTLC
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-APR-2025 13:22:51
Revision_Time = 27-SEP-2025 23:12:18
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 47
Total_Scans = 47
Relaxation_Delay = 2[s]
Recvr_Gain = 22
Temp_Get = 23[dC]
X_90_Width = 21.65[us]
X_Acq_Time = 0.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Ir_Atn_Dec = 33.47[dB]
Irr_Atn_Dec_Calc = 33.47[dB]
Irr_Atn_Noe = 33.47[dB]
O
O
O
O
tBu
F
tBuO
O
(thousandths)
X : parts per Million : Carbon13
197.341
167.930
167.859
166.842
164.309
133.360
133.331
130.784
130.688
115.619
115.403
81.494
81.460
77.321
77.000
76.683
58.372
42.799
29.312
27.844
27.791
17.499

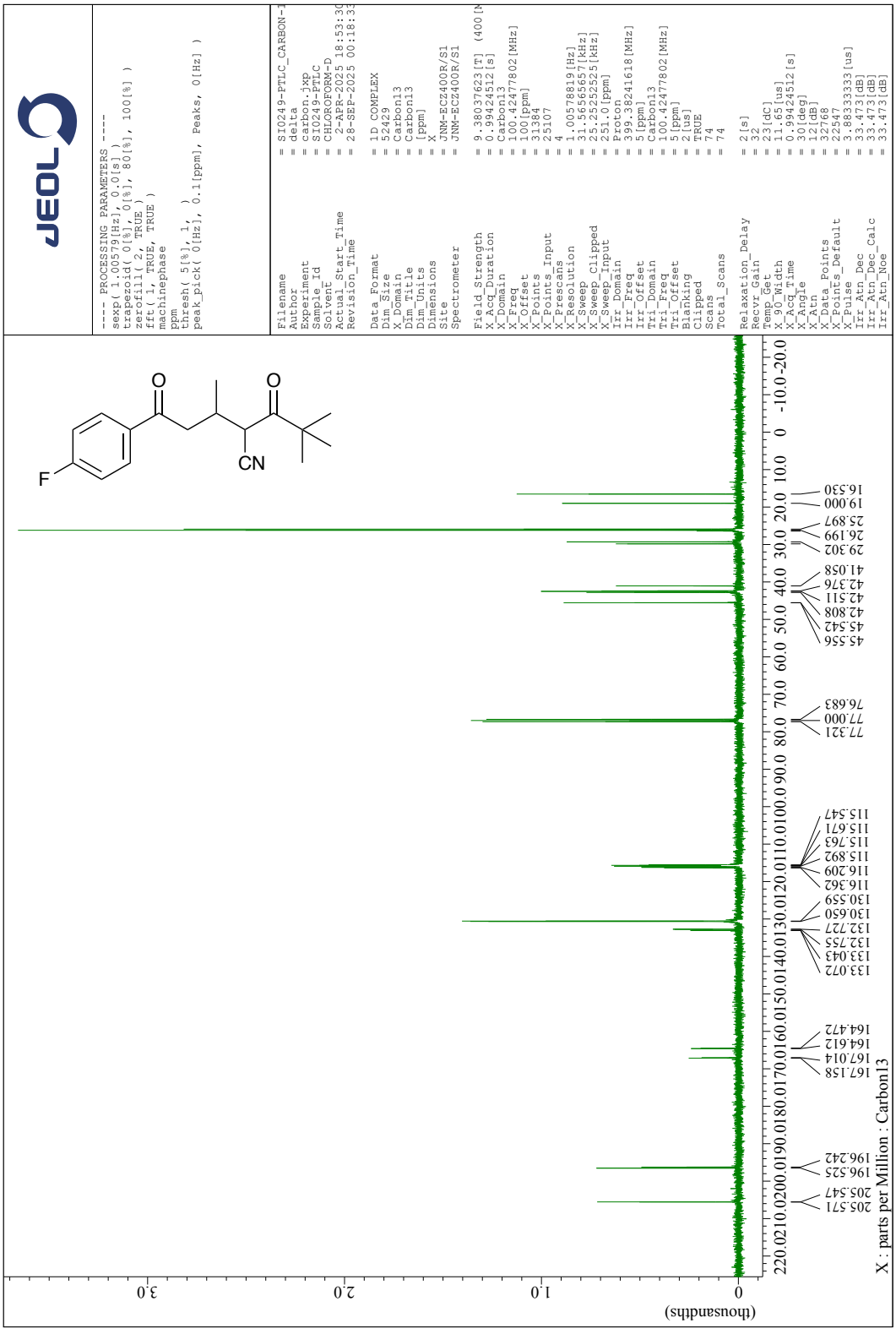
--- PROCESSING PARAMETERS ---
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.68062[ppm], -63.72[ppm])
reference(-63.62099[ppm], -63.72[ppm])
reference(-63.77864[ppm], -63.72[ppm])
thresh(82.15767[%], 1,)
以下に由来：: SI0256-PTLC_Fluorine-1-1.jdf
Filename = SI0256-PTLC_Fluorine
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0256-PTLC
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-APR-2025 18:43:02
Revision_Time = 27-SEP-2025 23:15:55
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.03380032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.6[dC]
X_90_Width = 2.05[us]
X_Acq_Time = 2.0338032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Ir_Mode = Off
Tri_Mode = Off
Date_Loop = 400
O
O
O
O
tBu
F
tBuO
PhCF3
-106.505
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-190.0
X : parts per Million : Fluorine19

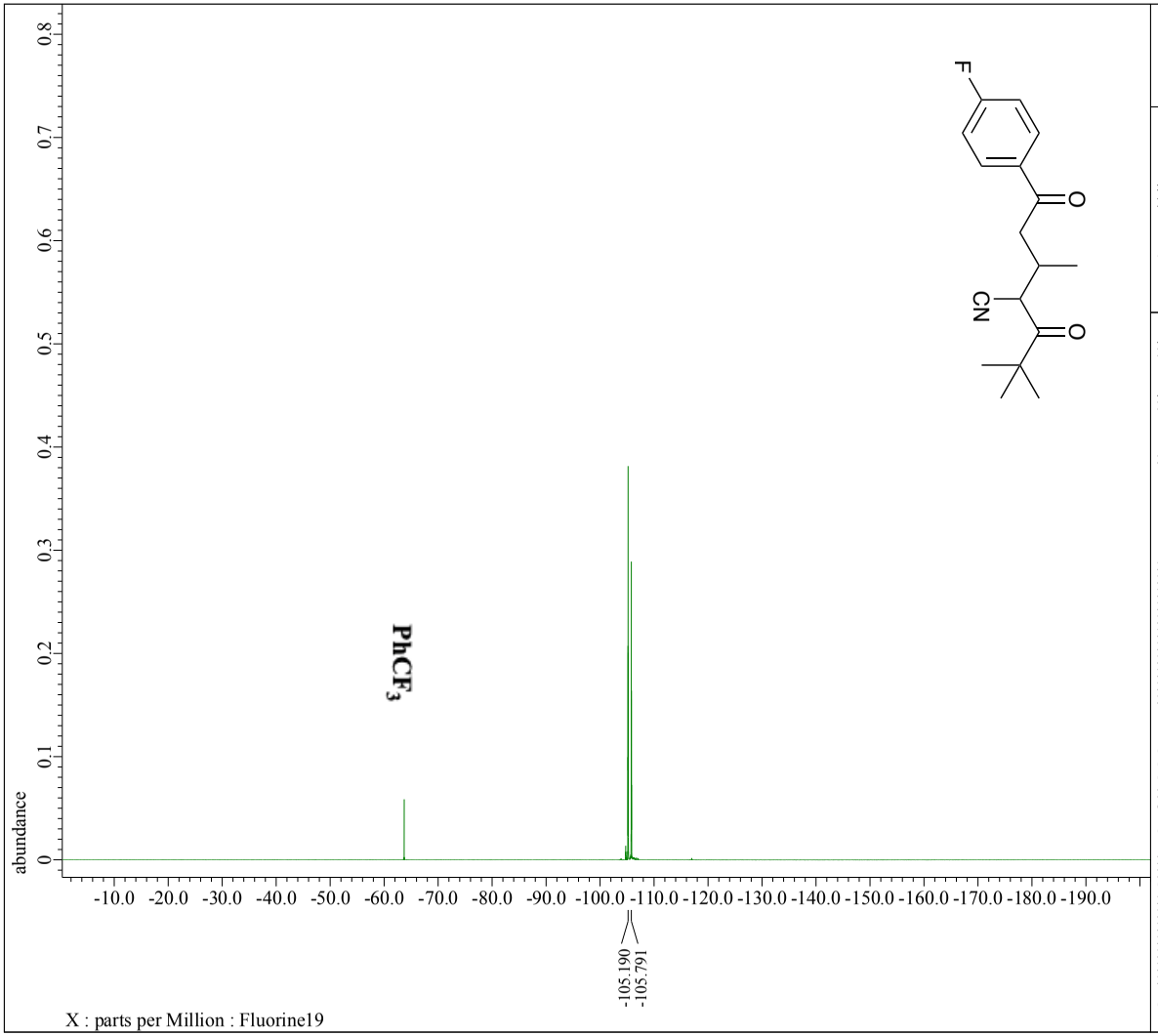

JEOL
--- PROCESSING PARAMETERS ---
sexp(0.25016[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.03969[ppm], 0[ppm])
thresh(9.70365[%], 1,)
Filename = SI0208-PTLC_PROT
Author = delta
Experiment = single_pulse_1H
Sample_Id = SI0208-PTLC-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-JAN-2025 19:(
Revision_Time = 22-SEP-2025 15:(
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.74735791[T] (5
X_Acq_Duration = 1.998745921[s]
X_Domain = Proton
X_Freq = 500.15991521[MHz
X_Offset = 5.0[ppm]
X_Points = 18757
X_Points_Input = 15005
X_Prescans = 0
X_Resolution = 0.50031372[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz
Tri_Offset = 5.0[ppm]
Blanking = 21us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.3[dC]
X_90_Width = 7.40[us]
X_Acq_Time = 1.998745921[s]
X_Angle = 45[deg]
X_Atn = 7.4[dB]
X_Data_Points = 32768
X_Points_Default = 31282
X_Pulse = 3.72[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
OEt
NO2
F
3.00
2.00
1.99
1.00
abundance
X : parts per Million : Proton


JEOL
---- PROCESSING PARAMETERS ----
sexp(1.00646[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
reference(77.15031[ppm], 0[ppm])
reference(-0.0[ppm], 77[ppm])
Filename = S10208-PTLC_CARE
Author = delco
Experiment = carbon.jxp
Sample_Id = S10208-PTLC-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-JAN-2025 19:1
Revision_Time = 22-SEP-2025 15:0
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC2500R/M3
Spectrometer = JNM-EC2500R/M3
Field_Strength = 11.74735579[T] (5
X_Acq_Duration = 0.99357984[s]
X_Domain = Carbon13
X_Freq = 125.765297.68[MHz
X_Offset = 100[ppm]
X_Points = 39303
X_Points_Input = 31442
X_Prescans = 4
X_Resolution = 1.00646164[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz
Irr_Offset = 5.0[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 65
Total_Scans = 65
Relaxation_Delay = 2[s]
Recvr_Gain = 52
Temp_Get = 22.4[dC]
X_90_Width = 11.26[us]
X_Acq_Time = 0.99357984[s]
X_Angle = 90[deg]
X_Atn = 32[dB]
X_Data_Points = 39557
X_Points_Default = 3.75333333[us]
Irr_Atn_Dec = 29.244[dB]
Irr_Atn_Dec_Calc = 29.244[dB]
Irr_Atn_Noe = 29.244[dB]
Irr_Bandwidth = 5.97826087[kHz]
Irr_Bandwidth_Ppm = 11.9526989[ppm]
Irr_Corresp_Pw90 = 92[us]
O
O
OEt
NO2
F
(thousandths)
X : parts per Million : Carbon13
195.762
195.688
166.899
166.880
164.866
164.847
163.717
132.860
132.836
130.685
130.669
130.611
130.594
115.860
115.844
115.685
115.668
91.124
90.803
77.254
77.000
76.746
62.900
62.866
40.736
40.635
30.523
30.494
16.293
16.094
13.824
13.795

---- PROCESSING PARAMETERS ----
sexp(0.49169[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-62.58738[ppm], -63.72[ppm])
thresh(82.78921[%], 1,)
Filename = SI0208-PTLC_Fluorine
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0208-PTLC
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-FEB-2025 20:05:46
Revision_Time = 22-SEP-2025 15:15:54
Data_Format = 1D COMPLEX
Dim_Size = 419430
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.0338032[s]
X_Domain = Fluorine19
X_Freq = 375.79488287[MHz]
X_Offset = -100[ppm]
X_Points = 192595
X_Points_Input = 154076
X_Prescans = 0
X_Resolution = 0.49168966[Hz]
X_Sweep = 94.6969697[kHz]
X_Sweep_Clipped = 75.75757576[kHz]
X_Sweep_Input = 201.0[ppm]
Irr_Domain = Fluorine19
Irr_Freq = 375.79488287[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.79488287[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 22
Temp_Get = 22.8[dC]
X_90_Width = 2.05[us]
X_Acq_Time = 2.0338032[s]
X_Angle = 45[deg]
X_Atn = 10[dB]
X_Data_Points = 65536
X_Points_Default = 65536
X_Pulse = 4.295[us]
Ir_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
O
O
OEt
NO2
F
PhCF3
-105.523
-105.598
abundance
0
0.1
0.2
0.3
0.4
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
X : parts per Million : Fluorine19


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-0.23732, 1.19173, 75.31759[%])
reference(-0.06721[ppm], 0[ppm])
reference(0.01489[ppm], 0[ppm])
thresh(0.57925[%], 1,)
Filename = SI0249-PTLC_PROTON-1
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SI0249-PTLC
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-APR-2025 18:50:04
Revision_Time = 28-SEP-2025 00:13:31
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 2.04870432[s]
X_Domain = Proton
X_Freq = 399.38241618[MHz]
X_Offset = 5[ppm]
X_Points = 15353
X_Points_Input = 12282
X_Prescans = 0
X_Resolution = 0.48811338[Hz]
X_Sweep = 7.49400048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
X_Sweep_Input = 15[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.38241618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 4[s]
Recvr_Gain = 42
Temp_Get = 23[dC]
X_90_Width = 8.8[us]
X_Acq_Time = 2.04870432[s]
X_Angle = 45[deg]
X_Atn = 9[dB]
X_Data_Points = 65536
X_Points_Default = 23890
X_Pulse = 3.4355[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 400
F
O
O
CN
9.00
3.00
2.00
2.00
1.00
0.57
0.43
0.58
0.42
8.020
8.016
8.006
8.003
7.997
7.995
7.984
7.981
7.178
7.173
7.165
7.156
7.144
7.140
7.135
7.122
4.351
4.340
4.121
4.106
3.178
3.157
3.046
3.033
3.027
2.988
2.983
1.299
1.257
1.224
1.212
1.195
1.164
1.147
abundance
X : parts per Million : Proton


JEOL
--- PROCESSING PARAMETERS ---
sexp(1.00579[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])
Filename = SI0249-PTLC_CARBON-1
Author = delta
Experiment = Carbon.jxp
Sample_Id = SI0249-PTLC
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-APR-2025 18:53:3
Revision_Time = 28-SEP-2025 00:18:3
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECZ400R/S1
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.38037623[T] (400[M
X_Acq_Duration = 0.99424512[s]
X_Domain = Carbon13
X_Freq = 100.42477802[MHz]
X_Offset = 100[ppm]
X_Points = 31384
X_Points_Input = 25107
X_Prescans = 4
X_Resolution = 1.00578819[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
X_Sweep_Input = 251.0[ppm]
Irr_Domain = Proton
Irr_Freq = 399.38241618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Carbon13
Tri_Freq = 100.42477802[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Scans = 74
Total_Scans = 74
Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Get = 21.1[dC]
X_90_Width = 21.65[us]
X_Acq_Time = 0.99424512[s]
X_Angle = 30[deg]
X_Atn = 12[dB]
X_Data_Points = 32768
X_Points_Default = 22547
X_Pulse = 3.88333333[us]
Ir_Atn_Dec = 33.47[dB]
Ir_Atn_Dec_Calc = 33.47[dB]
Irr_Atn_Noe = 33.47[dB]
O
O
CN
F
205.571
205.547
196.525
196.242
167.158
167.014
164.612
164.472
133.072
133.043
132.755
132.727
130.650
130.559
116.362
116.209
115.892
115.763
115.671
115.547
77.321
77.000
76.683
45.556
45.542
42.808
42.511
42.376
41.058
29.302
26.199
25.897
19.000
16.530
X : parts per Million : Carbon13
(thousandths)




```
---- PROCESSING PARAMETERS ----
sexp( 0.49169[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -62.54749[ppm], -63.72[ppm] )
thresh( 75.40491[%], 1,  )

以下に由来：: SI0249-PTLC_Fluorine-1-1.jdf
```

Filename	= SI0249-PTLC_Fluorine
Author	= delta
Experiment	= single_pulse.jxp
Sample_Id	= SI0249-PTLC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-APR-2025 21:25:28
Revision_Time	= 30-SEP-2025 15:30:48
Data_Format	= 1D COMPLEX
Dim_Size	= 419430
X_Domain	= Fluorine19
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECZ400R/S1
Spectrometer	= JNM-ECZ400R/S1
Field_Strength	= 9.38037623[T] (400[M
X_Acq_Duration	= 2.0338032[s]
X_Domain	= Fluorine19
X_Freq	= 375.79488287[MHz]
X_Offset	= -100[ppm]
X_Points	= 192595
X_Points_Input	= 154076
X_Prescans	= 0
X_Resolution	= 0.49168966[Hz]
X_Sweep	= 94.6969697[kHz]
X_Sweep_Clipped	= 75.75757576[kHz]
X_Sweep_Input	= 201.0[ppm]
Irr_Domain	= Fluorine19
Irr_Freq	= 375.79488287[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 375.79488287[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 52
Temp_Get	= 22.9[dC]
X_90_Width	= 8.59[us]
X_Acq_Time	= 2.0338032[s]
X_Angle	= 45[deg]
X_Atn	= 10[dB]
X_Data_Points	= 65536
X_Points_Default	= 65536
X_Pulse	= 4.295[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400