[Supplementary Information]

Total Synthesis of (±)-Halichonine B

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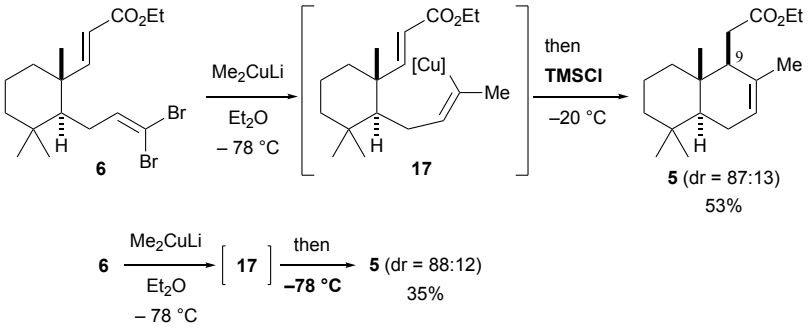
Table of Contents

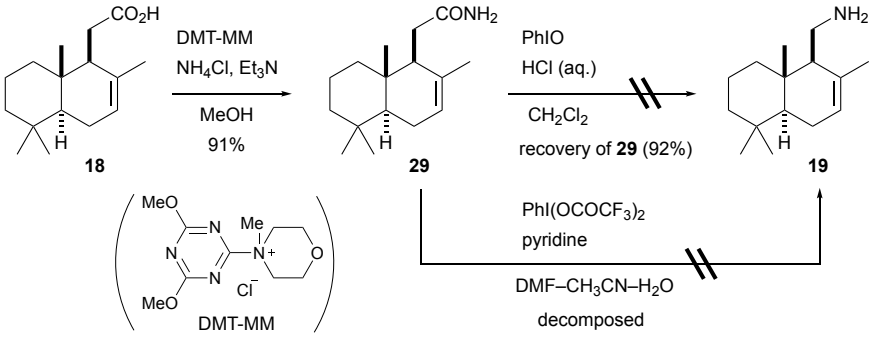
1. Supplementary schemes

Addition of TMSCl[1] in the methylative cyclization of **6** did not improve both yield and stereoselectivity of **5** (Scheme S1). Cyclization of **6** at –78 °C resulted in lower yield of **5** (35% yield) with similar stereoselectivity.



Scheme S1. Effects of additive and reaction temperature in the cyclization of dibromide **6**.

Attempts at Hofmann rearrangement of the primary carboxamide **29** derived from acid **18** did not proceed by using PhIO[2] with recovery of **29** (92% yield), whereas that by using $PhI(OCOCF_3)_2$[3] resulted in decomposition of **29** (Scheme S2).



Scheme S2. Attempted Hofmann rearrangement of carboxylic amide **29**.

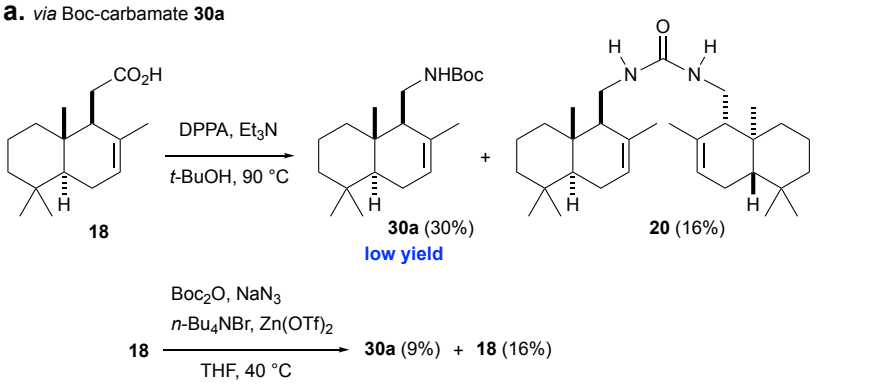
We also investigated a Curtius rearrangement-mediated two-step conversion from carboxylic acid **18** to amine **19** via the carbamate intermediates **30** (Scheme S3).

Trapping the isocyanate intermediate with *t*-BuOH gave Boc-carbamate **30a** in 30% yield with the undesired urea **20** (Scheme S3a). Conversion from **18** to **30a** by the Lebel and Leogane's procedure[4] using Boc_2O, NaN_3, and $Zn(OTf)_2$ gave inferior results.

Alternatively, Curtius rearrangement of **18** and subsequent treatment with 2,2,2-trichloroethanol produced Troc-carbamate **30b** only in 14% yield with urea **20** as a major product (50% yield) (Scheme S3b).

Curtius rearrangement of **18** and subsequent treatment with allyl alcohol efficiently gave Alloc-carbamate **30c** in 81% yield (Scheme S3c). However, deprotection of the Alloc group in **30c** resulted in low yield of amine **19** (<36% yield), probably due to high affinity of free amine **19** to the palladium center.

For the above reasons, we abandoned the conversion from **18** to **19** via the carbamate intermediates **30**.



Scheme S3. Attempted conversion of carboxylic acid **18** to primary amine **19** via carbamate intermediates **30**.

References for schemes S1–S3:

1. E. Nakamura, S. Matsuzawa, Y. Horiguchi and I. Kuwajima, *Tetrahedron Lett.*, 1986, **27**, 4029.
2. P. Liu, Z. Wang and X. Hu, *Eur. J. Org. Chem.*, 2012, 1994.
3. D. E. DeMong and R. M. Williams, *J. Am. Chem. Soc.*, 2003, **125**, 8561.
4. H. Lebel and O. Leogane, *Org. Lett.,* 2005, **7**, 4107.

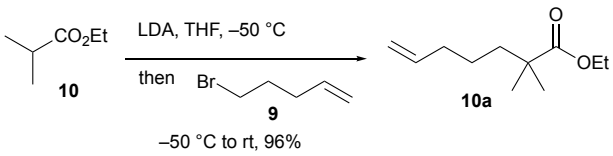
2. General information

All reactions were carried out in an oven-dried round-bottomed flask with an appropriate number of necks or test tube under an argon atmosphere. All vessels were first evacuated by a rotary pump and then flushed with argon prior to use. Analytical thin-layer chromatography (TLC) was performed on 0.25 mm E. Merck Silica gel (60F-254) plates. Reaction components were visualized by illumination with ultraviolet light (254 nm) and by staining with 6% ethanolic *p*-anisaldehyde (includes 6% conc. sulfuric acid and 1% acetic acid), 8% ethanolic phosphomolybdic acid, ceric ammonium molybdate in 10% sulfuric acid, or basic potassium permanganate solution. Fuji Sylysia silica gel PSQ 60B or PSQ 100B were used for flash column chromatography. Al_2O_3 column chromatography was performed on Sigma–Aldrich Aluminum oxide activated, basic, Brockmann I.

Anhydrous toluene, *N*,*N*-dimethylformamide (DMF), dichloromethane (CH_2Cl_2), diethyl ether (Et_2O), and tetrahydrofuran (THF) were purchased from Kanto Chemical Co., Inc. and further purified by passing through a solvent purification system (GlassContour) just prior to use. Anhydrous acetonitrile was purchased from Kanto Chemical Co., Inc. and further dried over MS3A. All other reagents and solvents were used as received from commercial sources without further purification unless otherwise noted.

Nuclear magnetic resonance (NMR) spectra were measured on a JEOL ECZ-500 spectrometer (^{1}H NMR: 500 MHz, ^{13}C{^{1}H} NMR: 125 MHz) in deuterated solvents. Chemical shifts for ^{1}H NMR spectra are reported in parts per million (ppm) by reference to tetramethylsilane (δ_H 0.00) or the residual solvent signal (δ_H 7.26 in $CDCl_3$ and δ_H 3.30 in CD_3OD), and signals are expressed as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), and broad (br). Coupling constants (*J*) are reported in Hz. Chemical shifts for ^{13}C{^{1}H} NMR spectra were reported in ppm by reference to the residual solvent signal (δ_C 77.0 in $CDCl_3$ and δ_C 49.0 in CD_3OD). Infrared (IR) spectra were recorded on a JASCO FT/IR-4700. High resolution mass spectra (HRMS) were measured on a Bruker Daltonics micrOTOF spectrometer (ESI). X-ray crystallographic data was recorded on a Rigaku XtaLAB Synergy Diffractometer.

3. Experimental procedures and characterization data



Synthesis of compound 10a: To a stirred solution of *i*-Pr_2NH (16.2 mL, 115 mmol) in THF (300 mL) was added *n*-BuLi (2.6 M in hexane, 42.3 mL, 110 mmol) at 0 ºC, and the solution was stirred at 0 °C for 30 min. After cooled to –50 °C, ethyl isobutyrate (**9**) (13.4 mL, 100 mmol) was slowly added to the resulting LDA solution at –50 ºC. After stirred at the same temperature for 1.5 h, 5-bromo-1-pentene (**9**) (15.4 mL, 130 mmol) was added to the mixture. The resulting mixture was gradually warmed to room temperature and stirred for 24 h. The reaction mixture was quenched with saturated aqueous NH_4Cl. After the layers were separated, the aqueous layer was extracted with Et_2O. The combined organic layers were washed with brine, dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 7:1) afforded ester **10a** (17.6 g, 95.7 mmol, 96%) as a yellow oil.

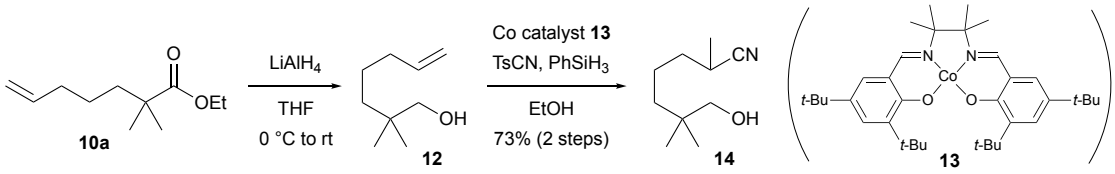
Data for 10a:

IR (film, cm^{-1}): 2978, 1728, 910.

^1H NMR (500 MHz, $CDCl_3$): 5.78 (ddt, J = 17.5, 10.5, 7.0 Hz, 1H), 5.00 (dd, J = 17.5, 1.5 Hz, 1H), 4.95 (dd, J = 10.5, 1.5 Hz, 1H), 4.11 (q, J = 7.1 Hz, 2H), 2.03 (q, J = 6.9 Hz, 2H), 1.54–1.50 (m, 2H), 1.35–1.28 (m, 2H), 1.24 (t, J = 7.2 Hz, 3H), 1.16 (s, 6H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 178.0, 138.6, 114.5, 60.2, 42.1, 40.1, 34.1, 25.1, 24.2, 14.2.

HRMS (ESI(+)): Calcd for $C_{11}H_{20}O_2Na$ $[M+Na]^+$ 207.1356, found 207.1361.



Synthesis of compound 14: To a mixture of $LiAlH_4$ (491 mg, 12.9 mmol) in THF (16 mL) was added dropwise a solution of ester **10a** (2.37 g, 12.9 mmol) in THF (10 mL) at 0 ºC. The mixture was stirred at room temperature for 2 h. The reaction mixture was quenched by successive addition of water (0.49 mL), 15% aqueous NaOH (0.49 mL), and H_2O (1.47 mL) at 0 °C. After stirred at room temperature for 30 min, the mixture was diluted with Et_2O, dried over $MgSO_4$, filtered through a pad of Celite (Et_2O rinse), and concentrated under reduced pressure. The crude alcohol **12** (1.54 g, colorless oil) was used for the next step without further purification.

To a mixture of the above crude ester **10a** (1.54 g), cobalt catalyst **13** (65.4 mg, 0.108 mmol), and TsCN (2.17 g, 11.9 mmol) in EtOH (53.9 mL) was added $PhSiH_3$ (1.34 mL, 10.8 mmol) at room temperature, and the mixture was stirred at this temperature for 3 h. The reaction mixture was concentrated under reduced pressure, and the residue was diluted with Et_2O (15 mL). The mixture was successively washed with saturated aqueous

$NaHCO_3$ (5mL) and brine (5 mL), dried over $MgSO_4$, and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 20:1 to 1:1) afforded nitrile **14** (1.59 g, 9.40 mmol, 73% for 2 steps) as a colorless oil.

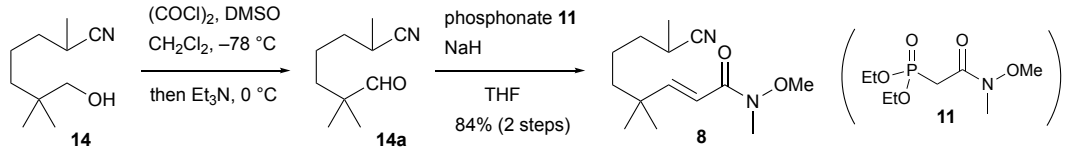
Data for 14:

IR (film, cm^{-1}): 3460, 2946, 2241, 1041.

^1H NMR (500 MHz, $CDCl_3$): 3.33 (br s, 2H), 2.67–2.59 (m, 1H), 1.65–1.34 (m, 5H), 1.32 (d, J = 7.4 Hz, 3H), 1.30–1.21 (m, 2H), 0.89 (s, 6H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 122.7, 70.8, 37.5, 34.6, 34.4, 25.0, 23.5, 21.1, 17.6.

HRMS (ESI(+)): Calcd for $C_{10}H_{19}NONa$ $[M+Na]^+$ 191.1359, found 192.1363.



Synthesis of compound 8: To a stirred solution of $(COCl)_2$ (5.8 mL, 67.4 mmol) in CH_2Cl_2 (50 mL) was slowly added a solution of DMSO (8.44 mL, 124 mmol) in CH_2Cl_2 (50 mL) at –78 °C. After stirred at –78 °C for 20 min, alcohol **14** (8.77 g, 51.8 mmol) in CH_2Cl_2 (160 mL) was added to the mixture at –78 °C, and the resulting mixture was stirred at the same temperature for 3 h. Et_3N (36.1 mL, 259 mmol) was added to the mixture. After stirred at –78 °C for 30 min, the resulting mixture was gradually warmed to 0 °C and stirred at this temperature for 30 min. The reaction mixture was quenched with H_2O (50 mL). After the layers were separated, the aqueous layer was extracted with Et_2O (three times). The combined organic layers were washed with H_2O and brine, dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. The crude aldehyde **14a** (9.53 g) was used for the following reaction without further purification.

To a mixture of NaH (60% dispersion in mineral oil, 1.56 g, 64.8 mmol) in THF (70 mL) was added slowly diethyl (*N*-methoxy-*N*-methylcarbamoylmethyl) phosphonate (**11**) (13.9 mL, 67.3 mmol) at 0 °C. After stirred at 0 °C for 30 min, the above crude aldehyde **14a** (9.53 g, as 51.8 mmol) in THF (59.5 mL) was added at 0 °C. The resulting mixture was stirred at room temperature for 3 h. The reaction mixture was quenched with saturated aqueous NH_4Cl and extracted with EtOAc. The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 10:1 to 1:1) afforded (*E*)-unsaturated amide **8** (11.0 g, 43.5 mmol, 84% for 2 steps) as a yellow oil.

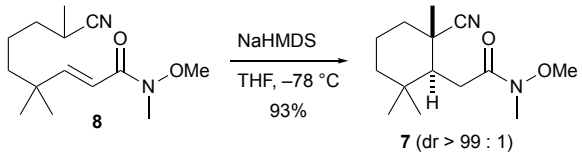
Data for 8:

IR (film, cm^{-1}): 2953, 2351, 1662, 1629, 1379, 1178, 1004.

^1H NMR (500 MHz, $CDCl_3$): 6.91 (d, J = 16.0 Hz, 1H), 6.30 (d, J = 16.0 Hz, 1H), 3.71 (s, 3H), 3.26 (s, 3H), 2.64–2.54 (m, 1H), 1.66–1.32 (m, 6H), 1.30 (d, J = 7.5 Hz, 3H), 1.09 (s, 6H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 166.7, 155.7, 122.6, 115.0, 61.3, 41.4, 36.3, 34.2, 32.0, 26.2, 26.1, 25.1, 21.9, 17.7.

HRMS (ESI(+)): Calcd for $C_{14}H_{24}N_2O_2Na^+$ $[M+Na]^+$ 275.1730, found 275.1733.



Synthesis of compound 7: To a solution of Weinreb amide **8** (11.0 g, 43.5 mmol) in THF (36 mL) was slowly added NaHMDS (1.9 M in THF, 34.3 mL, 65.3 mmol) at –78 °C over 50 min. The resulting mixture was stirred at –78 °C for 2.5 h. The reaction mixture was quenched with saturated aqueous NH_4Cl. After the layers were separated, the aqueous layer was extracted with EtOAc. The combined organic layers were dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 3:1 to 1:1) affordedcyclic nitrile **7** (10.3 g, 40.8 mmol, 93%, dr > 99:1) as a pale yellow oil.

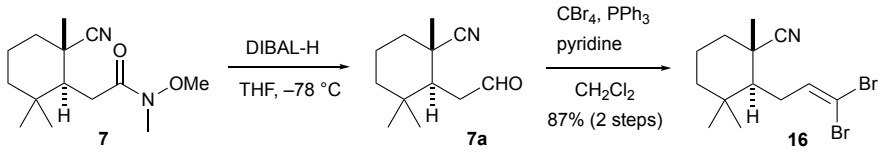
Data for 7:

IR (film, cm^{-1}): 2937, 2372, 2227, 1670, 1458, 1386, 999.

^1H NMR (500 MHz, $CDCl_3$): 3.75 (s, 3H), 3.21 (s, 3H), 2.66–2.61 (m, 1H), 2.49 (dt, J = 12.4, 4.9 Hz, 2H), 1.92–1.87 (m, 2H), 1.61–1.51 (m, 2H), 1.43 (dt, J = 13.7, 3.7 Hz, 1H), 1.39 (s, 3H), 1.36–1.30 (m, 1H), 0.94 (s, 3H), 0.91 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 172.7, 125.4, 60.8, 45.0, 39.3, 36.7, 36.2, 33.4, 32.0, 31.3, 29.5, 22.4, 19.9, 17.0.

HRMS (ESI(+)): Calcd for $C_{14}H_{24}N_2O_2Na^+$ $[M+Na]^+$ 275.1730, found 275.1733.



Synthesis of compound 16: To a solution of cyclic Weinreb amide **14** (577 mg, 2.28 mmol) in THF (4.5 mL) was slowly added diisobutylaluminum hydride (DIBAL-H, 1.0 M in toluene, 3.0 mL, 3.00 mmol) at –78 °C, and the mixture was stirred at –78 °C for 3 h. The reaction mixture was quenched by dropwise addition of EtOAc (3.5 mL) at –78 °C, and the mixture was stirred at this temperature for 20 min. Then, to the mixture was added a saturated aqueous sodium potassium tartrate solution (5 mL) at –78 °C, and the mixture was vigorously stirred at room temperature until both phases became clear (ca. 1.5 h). After the layers were separated, the aqueous layer was extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The crude aldehyde **7a** (564 mg, white powder) was used for the next step without further purification.

To a mixture of CBr_4 (1.132 g, 2.28 mmol), PPh_3 (1.86 g, 7.09 mmol) in CH_2Cl_2 (10 mL) was added pyridine (0.70 mL, 9.12 mmol) at 0 °C, and the mixture was stirred at this temperature for 5 min. To the mixture was added a solution of the above crude aldehyde **7a** (56 4 mg, as 2.28 mmol) in CH_2Cl_2 (5 mL) at 0 °C. After stirred at room temperature for 4 h, the reaction mixture was quenched with a saturated aqueous $NaHCO_3$ solution. After the layers were separated, the aqueous layer was extracted with Et_2O. The combined organic

layers were washed successively with brine, 5% aqueous $KHSO_4$ solution (four times), brine, dried over $MgSO_4$, and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 6:1 to 4:1) afforded dibromoalkene **16** (690 mg, 1.98 mmol, 87% for 2 steps) as a yellow solid.

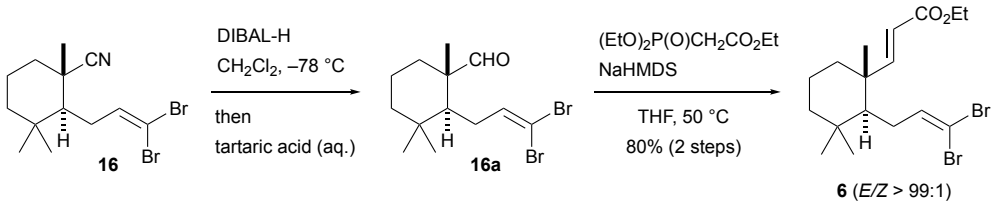
Data for 16:

IR (film, cm^{-1}): 2900, 2229, 1462, 1384, 848, 790.

^1H NMR (500 MHz, $CDCl_3$): 6.56 (dd, J = 7.7, 6.3 Hz, 1H), 2.43 (ddd, J = 16.2, 7.7, 6.3 Hz, 1H), 2.26 (ddd, J = 16.2, 6.3, 6.3 Hz, 1H), 1.99–1.93 (m, 1H), 1.87–1.80 (m, 1H), 1.72 (t, J = 6.3 Hz, 1H), 1.57–1.50 (m, 1H), 1.48–1.43 (m, 1H), 1.38 (s, 3H), 1.32–1.23 (m, 2H), 0.99 (s, 3H), 0.92 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 138.6, 126.2, 88.9, 49.9, 40.7, 38.2, 36.5, 34.1, 32.9, 32.1, 22.3, 19.4, 17.2.

HRMS (ESI(+)): Calcd for $C_{13}H_{19}Br_2NNa^+$ $[M+Na]^+$ 369.9776, found 369.9717.



Synthesis of compound 6: To a solution of nitrile **16** (469 mg, 1.34 mmol) in CH_2Cl_2 (6.8 mL) was slowly added DIBAL-H (1.0 M in hexane, 2.02 mL, 2.02 mmol) at –78 °C, and the mixture was stirred at –78 °C for 1.5 h. The reaction mixture was quenched by dropwise addition of EtOAc (2 mL) at –78 °C, and the mixture was stirred at –78 °C for 13 h. Then, to the mixture was added a 10% aqueous tartaric acid solution (20 mL) at –78 °C, and the mixture was stirred vigorously at room temperature until both phases became clear (ca. 2.5 h). After the layers were separated, the aqueous layer was extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, concentrated under reduced pressure. The residue was then dried by azeotropic removal of water with benzene. The crude aldehyde **16a** (471 mg, yellow oil) was used for the next step without further purification.

To a solution of triethyl phosphonoacetate (0.536 mL, 2.68 mmol) in THF (2 mL) was slowly added NaHMDS (1.9 M in THF, 1.34 mL, 2.54 mmol) at 0 °C. After the mixture was stirred at 0 °C for 30 min, to the mixture was added a solution of the above crude aldehyde **16a** (471 mg, as 1.34 mmol) in THF (4.7 mL) at 0 °C. After stirred at 50 °C for 24 h, the reaction mixture was quenched with a saturated aqueous NH_4Cl solution (8 mL) at room temperature. After the layers were separated, the aqueous layer was extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 20:1) afforded (*E*)-unsaturated ester **6** (452 mg, 1.07 mmol, 80% for 2 steps) as a yellow oil.

Data for 6:

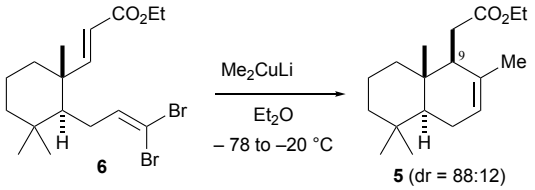
IR (film, cm^{-1}): 2927, 1716, 1643, 1462, 1388, 1273, 1037, 794.

^1H NMR (500 MHz, $CDCl_3$): 6.79 (d, J = 16.0 Hz, 1H), 6.29 (t, J = 7.4 Hz, 1H), 5.72 (d, J = 16.0 Hz, 1H),

4.20 (q, J = 7.5 Hz, 2H), 2.20–2.13 (m, 1H), 1.99–1.92 (m, 1H), 1.60–1.44 (m, 3H), 1.38–1.20 (m, 4H), 1.32 (t, J = 7.5 Hz, 3H), 1.11 (s, 3H), 0.93 (s, 6H).

$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): 167.0, 160.3, 140.3, 117.7, 87.9, 60.2, 52.3, 42.0, 41.3, 39.5, 34.0, 33.7, 31.4, 22.1, 18.3, 17.6, 14.3.

HRMS (ESI(+)): Calcd for $C_{17}H_{26}Br_2O_2Na^+$ $[M+Na]^+$ 443.0192, found 443.0189.



Synthesis of compound 5: Commercially available copper (I) iodide (95.0+%, purchased from FUJIFILM Wako Chemicals) was purified according to the literature procedure (G. B. Kauffman and L. Y. Fang, *Inorg. Synth.*, 1983, **22**, 101.) and stored in the dark under argon atmosphere.

To a mixture of the purified CuI (984 mg, 5.18 mmol) in freshly purified Et_2O (1.2 mL) was slowly added MeLi (1.04 M in Et_2O, 9.95 mL, 10.4 mmol) at 0 °C over 15 min, and the mixture was stirred at 0 °C for 30 min. To the resulting Me_2CuLi solution was added dropwise a solution of (*E*)-unsaturated ester **6** (437 mg, 1.04 mmol) in freshly purified Et_2O (3.0 mL + 1.0 mL rinse) at –78 °C over 10 min via cannula, and the mixture was stirred at –78 °C for 1 h. Then, the reaction mixture was gradually warmed to –20 °C over 20 min, and the mixture was stirred at –20 °C for additional 2 h. The reaction mixture was quenched with saturated aqueous NH_4Cl (10 mL) and 25% aqueous NH_3 (10 mL) at –20 °C, and the mixture was stirred vigorously at room temperature until the aqueous layer became clear dark blue. After the layers were separated, the aqueous layer was extracted with Et_2O (three times). The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/Et_2O = 30:1) afforded ester **5** (238 mg, 0.855 mmol, 83%, dr = 88:12) as a yellow oil.

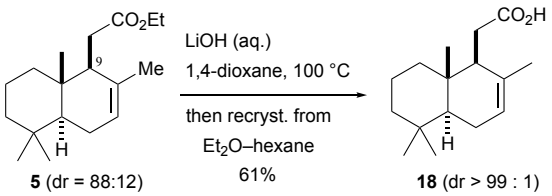
Data for major isomer of 5:

IR (film, cm^{-1}): 2927, 1720, 1643, 1458, 1369, 1261, 1172, 1037, 806.

^{1}H NMR (500 MHz, $CDCl_3$): 5.44–5.41 (m, 1H), 4.20–4.11 (m, 2H), 2.49 (d, J = 9.7 Hz, 1H), 2.38 (dd, J = 16.6, 2.9 Hz, 1H), 2.15 (dd, J = 16.9, 3.2 Hz, 1H), 2.07–1.94 (m, 1H), 1.88–1.80 (m, 1H), 1.75–1.66 (m, 1H), 1.57–1.55 (m, 3H), 1.54–1.39 (m, 3H), 1.30–1.24 (m, 1H), 1.26 (t, J = 7.2 Hz, 3H), 1.18 (ddd, J = 13.4, 13.4, 3.6 Hz, 1H), 1.09 (ddd, J = 13.2, 13.2, 4.0 Hz, 1H), 0.88 (s, 3H), 0.87 (s, 3H), 0.75 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): 174.8, 133.8, 122.6, 60.3, 50.4, 49.7, 42.0, 39.0, 35.9, 33.1, 32.9, 32.6, 23.7, 21.8, 21.4, 18.7, 14.1, 13.9.

HRMS (ESI(+)): Calcd for $C_{18}H_{30}O_2K^+$ $[M+K]^+$ 317.1877, found 317.1839.



5 (dr = 88:12) **18** (dr > 99 : 1)

Synthesis of compound 18: To a solution of ester **5** (389 mg 1.40 mmol, dr = 88:12) in 1,4-dioxane (7.0 mL) was added saturated aqueous LiOH (7.0 mL) at room temperature, and the mixture was vigorously stirred at the 100 °C for 48 h. After cooled to room temperature, the reaction mixture was acidified with 5% aqueous $KHSO_4$ at room temperature. After the layers were separated, the aqueous layer was extracted with EtOAc (three times). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. Recrystallization of the crude acid (348 mg, white powder) from Et_2O–hexane (1/5) gave pure carboxylic acid **18** (212 mg, 0.846 mmol, 61%, dr > 99:1) as a white solid.

Further recrystallization of **18** from EtOAc afforded colorless needles, which were analyzed by X-ray crystallographic analysis.

Data for 18:

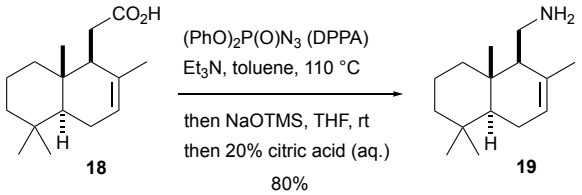
IR (film, cm^{-1}): 2924, 2359, 2339, 2339, 1731, 1698, 1651, 1539, 1455.

^1H NMR (500 MHz, $CDCl_3$): 5.46–5.42 (m, 1H), 2.51–2.42 (m, 2H), 2.21 (dd, J =17.2, 9.7 Hz, 1H), 2.00 (d, J = 17.8 Hz, 1H), 1.89–1.80 (m, 1H), 1.73 (d, J = 12.0 Hz, 1H), 1.61 (s, 3H), 1.59–1.39 (m, 3H), 1.28 (dd, J =12.0, 4.6 Hz, 1H), 1.18 (ddd, J =13.1, 13.1, 4.0 Hz, 1H), 1.09 (ddd, J = 13.1, 13.1, 4.0 Hz, 1H), 0.89 (s, 3H), 0.87 (s, 3H), 0.76 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 181.6, 133.4, 122.9, 50.4, 49.7, 42.0, 39.1, 35.9, 33.1, 32.9, 32.4, 23.7, 21.8, 21.4, 18.7, 13.9.

HRMS (ESI(+)): Calcd for $C_{16}H_{26}O_2Na^+$ $[M+Na]^+$ 273.1825, found 273.1818.

Mp: 145–147 °C (EtOAc).



18 **19**

Synthesis of 19: To a solution of carboxylic acid **18** (60.4 mg, 0.241 mmol) in toluene (1.21 mL) were added Et_3N (50.4 µL, 0.362 mmol) and diphenylphosphoryl azide (DPPA) (77.8 µL, 0.362 mmol), and the reaction mixture was heated to reflux for 11 h. After cooled to rt, to the mixture was added a solution of sodium trimethylsilanolate (NaOTMS) (4.0 M in THF, 1.21 mL, 4.84 mmol), and the mixture was stirred at room temperature for 12 h. The reaction mixture was quenched with 20% aqueous citric acid. To the mixture was added 15% aqueous NaOH until the pH of the mixture was 11. The mixture was extracted with Et_2O (four times). The combined organic layers were washed successively with 15% aqueous NaOH and brine, dried over Na_2SO_4, and concentrated under reduced pressure. Purification by column chromatography on basic

Al_2O_3 ($CHCl_3$/MeOH = 1:0 to 5:1) gave amine **19** (42.5 mg, 0.188 mmol, 80%) as a yellow oil.

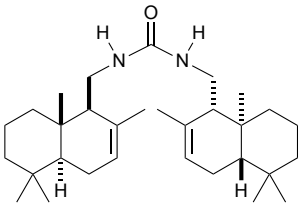
Data for 19:

IR (film, cm^{-1}): 2922, 2848, 1728, 1578, 1457, 1386, 1364, 1220.

^1H NMR (500 MHz, $CDCl_3$): 5.49–5.46 (m, 1H), 2.88 (dd, *J* = 13.2, 2.3 Hz, 1H), 2.68 (dd, *J* =13.2, 6.3 Hz, 1H), 2.01–1.91 (m, 2H), 1.89–1.81 (m, 1H), 1.77 (s, 3H), 1.71–1.67 (m, 1H), 1.60–1.39 (m, 5H), 1.20–1.13 (m, 2H), 1.06 (ddd, *J* = 13.2, 13.2, 3.4 Hz, 1H), 0.88 (s, 3H), 0.86 (s, 3H), 0.79 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 133.8, 123.4, 59.0, 49.9, 42.1, 40.0, 39.5, 36.4, 33.2, 32.9, 23.6, 22.1, 22.0, 18.7, 14.4.

HRMS (ESI(+)): Calcd for $C_{15}H_{28}N^+$ $[M+H]^+$ 222.2216, found 222.2219.



20

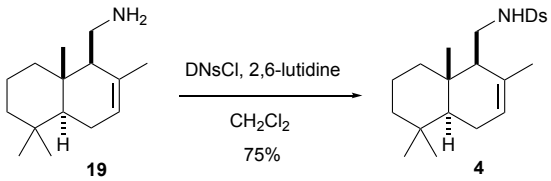
Data for compound 20:

IR (ATR, cm^{-1}): 3355, 3306, 2920, 2846, 1624, 1565, 1456, 1253, 638.

^1H NMR (500 MHz, $CDCl_3$): 5.53 (d, *J* = 4.6 Hz, 2H), 4.11–4.06 (m, 2H), 3.44–3.35 (m, 2H), 3.21–3.11 (m, 2H), 2.03–1.95 (m, 4H), 1.90–1.81 (m, 4H), 1.70 (s, 6H), 1.52–1.39 (m, 6H), 1.20–1.13 (m, 4H), 1.11–1.03 (m, 2H), 0.88 (s, 6H), 0.86 (s, 6H), 0.82 (s, 6H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 157.5, 132.7, 124.6, 54.8, 49.9, 42.0, 39.7, 38.6, 38.5, 36.3, 33.3, 32.9, 23.6, 22.0, 18.7, 14.4.

HRMS (ESI(+)): Calcd for $C_{31}H_{52}N_2ONa^+$ $[M+Na]^+$ 491.3977, found 491.3972.



19 **4**

Synthesis of compound 4: To a solution of amine **19** (39.1mg, 0.177 mmol) in CH_2Cl_2 (0.88 mL) were added 2,4-dinitrobenzenesulfonyl chloride (DNsCl) (70.6 mg, 0.265 mmol) and 2,6-lutidine (58.3 μL, 0.530 mmol) at room temperature. After stirred at room temperature for 6 h, the reaction mixture was quenched with 10% aqueous $KHSO_4$. After the layers were separated, the aqueous layer was extracted with CH_2Cl_2 (four times). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 93:17 to 15:1) afforded DNs-amide **4** (59.7 mg, 0.132 mmol, 75%) as a white solid.

Data for 4:

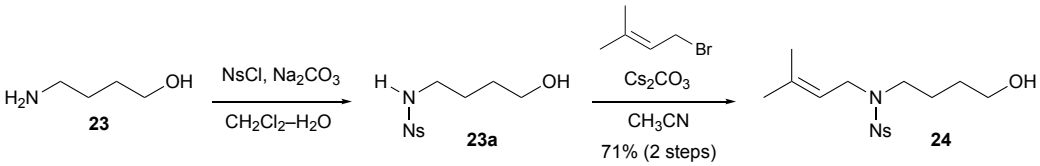
IR (film, cm^{-1}): 3747, 3671, 3380, 3103, 2923, 2849, 1552, 1349, 1170.

^{1}H NMR (500 MHz, $CDCl_3$): 8.68 (d, *J* = 2.5 Hz, 1H), 8.58 (dd, *J* = 8.5, 2.5 Hz, 1H), 8.37 (d, *J* = 8.5 Hz, 1H), 5.57–5.53 (m, 1H), 5.34 (t, *J* = 6.0 Hz, 1H), 3.36 (ddd, *J* = 12.6, 5.7, 2.9 Hz, 1H), 3.31 (ddd, *J* = 12.3, 5.7, 5.7 Hz, 1H), 2.00 (d, *J* = 17.2 Hz, 1H), 1.89–1.80 (m, 2H), 1.68 (s, 3H), 1.64–1.40 (m, 3H), 1.30–1.25 (m, 1H), 1.17–1.10 (m, 2H), 0.99 (ddd, *J* = 13.2, 13.2, 4.0 Hz, 1H), 0.87 (s, 3H), 0.85 (s, 3H), 0.79 (s, 3H).

^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): 149.8, 148.3, 139.0, 132.7, 130.8, 127.0, 125.6, 120.8, 54.5, 49.6, 42.0, 41.8, 39.6, 36.3, 33.2, 32.9, 23.4, 21.9, 21.7, 18.6, 14.5.

HRMS (ESI(−)): Calcd for $C_{21}H_{28}N_3O_6S_1^-$ $[M-H]^-$ 450.1704, found 450.1693.

Mp: 154–155 °C.



Synthesis of 24: To a solution of 4-amino-1-butanol (**23**) (0.928 mL, 10.0 mmol) in CH_2Cl_2 (20 mL) and water (20 mL) were added Na_2CO_3 (1.06 g, 10.0 mmol) and 2-nitrobenzenesulfonyl chloride (NsCl) (2.20 g, 9.93 mmol) at room temperature. The mixture was stirred at room temperature for 3 h. The reaction mixture was quenched with saturated aqueous NH_4Cl. After the layers were separated, the aqueous layer was extracted with CH_2Cl_2 (two times). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude Ns-amide **23a** (2.72 g, white solid) was used for the next step without further purification.

To a solution of the above crude Ns-amide **23a** (2.72 g) in CH_3CN (40 mL) were added Cs_2CO_3 (8.97 g, 27.5 mmol) and prenyl bromide (2.14 mL, 20.9 mmol) at room temperature. After stirred at room temperature for 17 h, the reaction mixture was diluted with H_2O (5 mL) and extracted with EtOAc (three times). The combined organic extracts were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 2:1 to 1:2) afforded alcohol **24** (2.41 g, 7.04 mmol,71% for 2 steps) as a yellow oil.

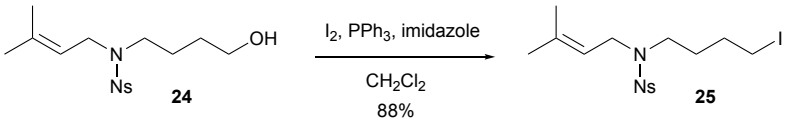
Data for 24:

IR (film, cm^{-1}): 3348, 2935, 1674, 1550, 1442, 1338, 1161, 1026, 852, 767, 586.

^{1}H NMR (500 MHz, $CDCl_3$): 8.00 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.72–7.60 (m, 3H), 5.06–5.00 (m, 1H), 3.91 (d, *J* = 6.9 Hz, 2H), 3.63 (t, *J* = 6.3 Hz, 2H), 3.30 (t, *J* = 7.4 Hz, 2H), 1.66 (s, 3H), 1.63 (s, 3H), 1.68–1.50 (m, 4H).

^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): 147.9, 137.5, 133.7, 133.3, 131.5, 130.6, 124.0, 118.5, 62.1, 46.8, 44.7, 29.4, 25.7, 24.4, 17.7.

HRMS (ESI(+)): Calcd for $C_{15}H_{22}N_2O_5SNa^+$ $[M+Na]^+$ 365.1142, found 365.1112.



Synthesis of 25: To a solution of alcohol **24** (1.36 g, 3.97 mmol) in CH_2Cl_2 (9.9 mL) were added PPh_3 (1.25 g, 4.77 mmol), imidazole (351 mg, 5.16 mmol), and iodine (56.6 mg, 0.125 mmol) at room temperature. After stirred at room temperature in the dark for 24 h, the reaction mixture was quenched with saturated aqueous Na_2SO_3 and extracted with CH_2Cl_2 (three times). The combined organic extracts were washed successively with H_2O and brine, dried over Na_2SO_4, and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc = 4:1) afforded alkyl iodide **25** (1.58 g, 3.49 mmol, 88%) as a yellow oil.

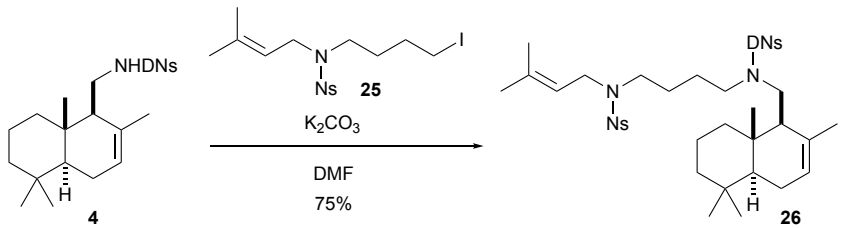
Data for 25:

IR (film, cm^{-1}): 3901, 3744, 2914, 1542, 1372, 1345, 1161.

^1H NMR (500 MHz, $CDCl_3$): 8.02 (dd, J = 6.9, 2.3 Hz, 1H), 7.71–7.62 (m, 3H), 5.05–5.00 (m, 1H), 3.91 (d, J = 6.9 Hz, 2H), 3.30 (t, J = 7.5 Hz, 2H), 3.18 (t, J = 6.9 Hz, 2H), 1.82–1.62 (m, 4H), 1.68 (s, 3H), 1.65 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 147.9, 137.7, 133.8, 133.3, 131.5, 130.8, 124.1, 118.5, 45.8, 44.8, 30.2, 28.8, 25.8, 17.9, 6.3.

HRMS (ESI(+)): Calcd for $C_{15}H_{21}N_2O_5SK^+$ $[M+K]^+$ 490.9896, found 490.9898.



Synthesis of compound 26: To a mixture of DNs-amide **4** (11.3 mg, 25.0 μmol) and K_2CO_3 (17.3 mg, 0.125 mmol) was added a solution of alkyl iodide **25** (56.6 mg, 0.125 mmol) in DMF (125 μL) at room temperature. After stirred at room temperature in the dark for 24 h, the reaction mixture was diluted with H_2O and extracted with Et_2O (three times). The combined organic extracts were washed successively with H_2O and brine, dried over Na_2SO_4, and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, hexane/EtOAc =4:1) afforded alkylation product **26** (14.5 mg, 18.6 μmol, 75 %) as a pale yellow solid.

Data for 26:

IR (film, cm^{-1}): 2923, 1541, 1455, 1349, 1162.

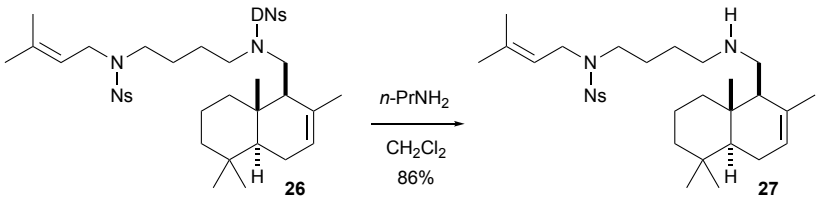
^1H NMR (500 MHz, $CDCl_3$): 8.52 (dd, J = 8.6, 2.3 Hz, 1H), 8.42 (d, J = 1.7 Hz, 1H), 8.21 (d, J = 8.6 Hz, 1H), 7.94 (dd, J = 8.6, 2.3 Hz, 1H), 7.71–7.64 (m, 2H), 7.61 (dd, J = 6.9, 2.3 Hz, 1H), 5.51–5.47 (m, 1H), 4.95–4.91 (m, 1H), 3.81 (d, J = 7.5 Hz, 2H), 3.58 (dd, J = 13.2, 9.2, Hz, 1H), 3.39–3.32 (m, 1H), 3.31–3.21 (m, 4H), 2.12–1.82 (m, 4H), 1.76 (s, 3H), 1.65 (s, 3H), 1.61 (s, 3H), 1.67–1.38 (m, 6H), 1.27–1.14 (m, 3H), 1.01 (ddd, J = 12.6, 12,6, 3.4 Hz, 1H), 0.89 (s, 3H), 0.88 (s, 3H), 0.84 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 149.7, 148.2, 147.9, 137.9, 137.5, 133.5, 133.4, 132.6, 132.5, 131.6, 130.8,

126.2, 124.5, 124.1, 119.6, 118.1, 49.9, 49.5, 47.8, 46.4, 46.2, 44.7, 41.8, 39.4, 36.5, 33.2, 33.1, 25.7, 25.4, 25.1, 23.5, 22.4, 22.0, 18.7, 17.7, 13.6.

HRMS (ESI(+)): Calcd for $C_{36}H_{49}N_5O_{10}S_2Na^+$ $[M+Na]^+$ 798.2813, found 798.2813.

Mp: 51–53 °C.



Synthesis of compound 27: To a solution of DNs-amide **26** (126 mg, 0.162 mmol) in CH_2Cl_2 (0.81 mL) was added *n*-propylamine (266 μL, 3.24 mmol) at room temperature. After stirred at room temperature for 25.5 h, the reaction mixture was concentrated under reduced pressure. Purification of the residue by flash column chromatography (SiO_2, $CHCl_3$/MeOH/Et_3N = 80:2:1) afforded secondary amine **27** (76.1 mg, 0.139 mmol, 86%) as a yellow oil.

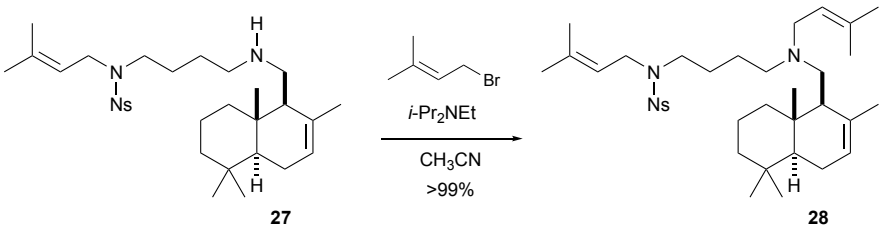
Data for 27:

IR (film, cm^{-1}): 3337, 2923, 2848, 2341, 1671, 1671, 1546, 1371, 1347, 1441, 1161.

^1H NMR (500 MHz, $CDCl_3$): 8.01 (dd, *J* = 5.7, 1.7 Hz, 1H), 7.70–7.63 (m, 2H), 7.61 (dd, *J* = 6.3, 1.7 Hz, 1H), 5.45-5.41 (m, 1H), 5.04 (t, *J* = 6.9 Hz, 1H), 3.91 (d, *J* = 6.9 Hz, 2H), 3.27 (t, *J* = 7.5 Hz, 2H), 2.67 (dd, *J* = 11.5, 1.2 Hz, 1H), 2.60 (ddd, *J* = 11.5, 6.9, 6.9 Hz, 1H), 2.51 (ddd, *J* = 12.0, 6.9, 6.9 Hz, 1H), 2.44 (ddd, *J* = 12.0, 6.9, 6.9 Hz, 1H), 2.00–1.80 (m, 3H), 1.71 (s, 3H), 1.67 (s, 3H), 1.62 (s, 3H), 1.60–1.38 (m, 8H), 1.20–1.12 (m, 2H), 1.05 (ddd, *J* = 9.7, 9.7, 3.4 Hz, 1H), 0.88 (s, 3H), 0.85 (s, 3H), 0.76 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 148.0, 137.5, 134.0, 133.4, 133.2, 131.5, 130.8, 124.1, 123.4, 118.6, 54.5, 49.8, 49.2, 47.8, 46.8, 44.8, 42.1, 39.2, 36.2, 33.2, 32.9, 26.2, 25.9, 25.8, 23.7, 22.0, 21.9, 18.7, 17.8, 13.9.

HRMS (ESI(+)): Calcd for $C_{30}H_{48}N_3O_4S^+$ $[M+H]^+$ 546.3374, found 546.3360.



Synthesis of compound 28: To a stirred solution of secondary amine **27** (21.5 mg, 39.4 μmol) in CH_3CN (197 μL) were added *i*-Pr_2NEt (6.86 μL, 39.4 μmol) and prenyl bromide (5.01 μL, 43.3 μmol) at room temperature. After stirred at room temperature for 13 h, the reaction mixture was diluted with H_2O and extracted with EtOAc (four times). The combined organic extracts were dried over Na_2SO_4 and concentrated. The residue was purified by column chromatography on basic Al_2O_3 (hexane/Et_2O = 19:1 to 3:1) to give

tertiary amine **28** (24.3 mg, 39.4 μmol, >99%) as a yellow oil.

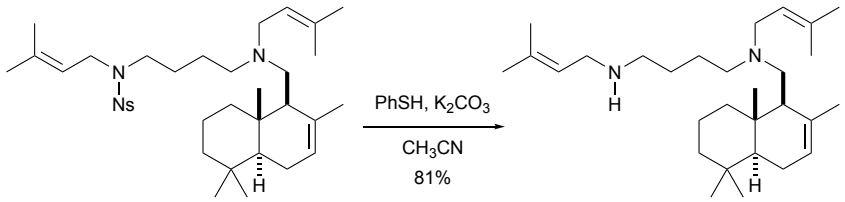
Data for 28:

IR (film, cm^{-1}): 2922, 2852, 1544, 1440, 1372, 1349, 1161.

^1H NMR (500 MHz, $CDCl_3$): 8.01 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.69–7.62 (m, 2H), 7.61 (dd, *J* = 6.9, 2.3 Hz, 1H), 5.38 (d, *J* = 4.0 Hz, 1H), 5.21–5.17 (m, 1H), 5.06–5.02 (m, 1H), 3.90 (d, *J* = 6.9 Hz, 2H), 3.25 (t, *J* = 7.5 Hz, 2H), 3.06 (dd, *J* = 14.3, 5.7 Hz, 1H), 2.80 (dd, *J* = 14.3, 8.0 Hz, 1H), 2.47 (ddd, *J* = 13.1, 7.5, 7.5 Hz, 1H), 2.30–2.21 (m, 2H), 2.20–2.13 (m, 1H), 2.02–1.92 (m, 2H), 1.87–1.77 (m, 2H), 1.72 (s, 3H), 1.71 (s, 3H), 1.67 (s, 3H) 1.62 (s, 3H), 1.61 (s, 3H), 1.60–1.30 (m, 7H), 1.22–1.13 (m, 2H), 0.98 (ddd, *J* = 12.6, 12.6, 3.4 Hz, 1H), 0.87 (s, 3H), 0.86 (s, 3H), 0.72 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 148.0, 137.2, 136.0, 134.2, 134.0, 133.1, 131.4, 130.8, 124.1, 121.9, 121.8, 118.9, 53.7, 52.9, 51.5, 51.1, 50.2, 47.1, 44.7, 42.3, 39.1, 36.1, 33.3, 33.0, 26.2, 25.9, 25.8, 24.1, 23.7, 22.5, 22.0, 18.8, 17.9, 17.7, 13.6.

HRMS (ESI(+)): Calcd for $C_{35}H_{56}N_3O_4S^+$ $[M+H]^+$ 614.3988, found 614.3986.



28 (±)-halichonine B (**2**)

Synthesis of (±)-halichonine B (2): To a solution of tertiary amine **28** (19.9 mg, 32.4 μmol) in CH_3CN (0.162 mL) were added PhSH (4.30 μL, 42.1 μmol) and K_2CO_3 (5.82 mg, 42.1 μmol) at room temperature, and the mixture was stirred at 40 °C for 14 h. After cooled to room temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ and extracted with EtOAc (three times). The combined organic extracts were dried over Na_2SO_4 and concentrated. The residue was purified by column chromatography on basic Al_2O_3 (CH_2Cl_2/MeOH = 98:2) to give (±)-halichonine B (**2**) (11.2 mg, 26.1 μmol, 81%) as a yellow oil.

Data for synthetic (±)-halichonine B (2):

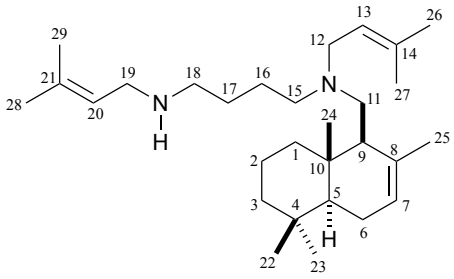
IR (film, cm^{-1}): 2923, 2853, 1731, 1671, 1557, 1454.

^1H NMR (500 MHz, CD_3OD): 5.38–5.35 (m, 1H), 5.28–5.21 (m, 2H), 3.19 (d, *J* = 6.9 Hz, 2H), 3.13 (dd, *J* = 14.0, 6.3 Hz, 1H), 2.88 (dd, *J* = 14.0, 7.5 Hz, 1H), 2.60–2.52 (m, 3H), 2.37–2.29 (m, 2H), 2.27–2.22 (m, 1H), 2.08–2.02 (m, 1H), 2.01–1.94 (m, 1H), 1.90–1.82 (m, 2H), 1.75 (s, 3H), 1.73 (s, 3H), 1.71 (s, 3H), 1.66 (s, 3H), 1.64 (s, 3H), 1.63–1.40 (m, 7H), 1.24–1.16 (m, 2H), 1.04 (ddd, *J* = 12.6, 12.6, 4.0 Hz, 1H), 0.89 (s, 3H), 0.86 (s, 3H), 0.75 (s, 3H).

$^{13}C\{^1H\}$ NMR (125 MHz, CD_3OD): 136.9, 135.9, 135.2, 123.1, 123.0, 54.9, 54.5, 53.1, 52.3, 51.7, 50.0, 47.6, 43.5, 40.5, 37.4, 34.0, 33.9, 28.5, 26.1, 26.0, 25.8, 24.8, 22.9, 22.4, 19.9, 18.1, 18.0, 14.2.

HRMS (ESI(+)): Calcd for $C_{29}H_{53}N_2^+$ $[M+H]^+$ 429.4213, found 429.4203.

4. Comparison of ^{1}H NMR and ^{13}C NMR spectra between natural and synthetic halichonine B (2)



halichonine B (**2**)

Table S1. Comparison of ^{1}H NMR spectra of natural halichonine B (**2**) by Suenaga–Uemura group, and synthetic halichonine B (**2**) by Hayakawa–Kigoshi, Li, and our groups.

Carbon No.	^{1}H NMR (CD_3OD)			
	Chemical shifts in ppm (multiplicity, *J* [Hz])			
	Suenaga–Uemura (600 MHz)[a]	Hayakawa–Kigoshi (600 MHz)[b]	Li (500 MHz)[c]	This synthesis (500 MHz)
1a	1.01 (m)	1.03 (ddd, 13.1, 13.1, 3.3)	1.07–1.00 (m)	1.04 (ddd, 12.6, 12.6, 4.0)
1b	2.03 (m)	2.04 (br m)	2.08–2.03 (m)	2.08–2.02 (m)
2a	1.39 (m)	1.61–1.36 (m)	1.51–1.44 (m)	1.63–1.40 (m)
2b	1.55 (m)	1.61–1.36 (m)	1.60–1.56 (m)	1.63–1.40 (m)
3a	1.16 (m)	1.23–1.16 (m)	1.24–1.17 (m)	1.24–1.16 (m)
3b	1.38 (m)	1.61–1.36 (m)	1.44–1.40 (m)	1.63–1.40 (m)
4	—	—	—	—
5	1.18 (m)	1.23–1.16 (m)	1.24–1.17 (m)	1.24–1.16 (m)
6	1.95 (m, 2H)	1.90–1.80 (m, 2H)	1.91–1.82 (m, 2H)	1.90–1.82 (m, 2H)
7	5.34 (s)	5.36 (m)	5.39–5.36 (m)	5.38–5.35 (m)
8	—	—	—	—
9	1.84 (m)	1.96 (br m)	2.00–1.94 (m)	2.01–1.94 (m)
10	—	—	—	—
11	2.31 (m, 2H)	2.36–2.28 (m, 2H)	2.37–2.29 (m, 2H)	2.37–2.29 (m, 2H)
12a	2.86 (dd, 7.8, 13.9)	2.88 (dd, 14.1, 7.7)	2.89 (dd, 14.2, 7.7)	2.88 (dd, 14.0, 7.5)
12b	3.11 (dd, 5.7, 13.9)	3.13 (dd, 14.1, 6.1)	3.14 (dd, 14.2, 6.2)	3.13 (dd, 14.0, 6.3)
13	5.22 (m)	5.28–5.20 (m)	5.28–5.23 (m)	5.28–5.21 (m)
14	—	—	—	—
15a	2.22 (m)	2.27–2.20 (m)	2.27–2.22 (m)	2.27–2.22 (m)
15b	2.52 (m)	2.59–2.51 (m)	2.61–2.53 (m)	2.60–2.52 (m)

16	1.43 (m, 2H)	1.61–1.36 (m, 2H)	1.51–1.44 (m, 2H)	1.63–1.40 (m, 2H)
17	1.45 (m, 2H)	1.61–1.36 (m, 2H)	1.55–1.51 (m) 1.51–1.44 (m)	1.63–1.40 (m, 2H)
18	2.55 (m, 2H)	2.59–2.51 (m, 2H)	2.61–2.53 (m, 2H)	2.60–2.52 (m, 2H)
19	3.18 (d, 6.5, 2H)	3.18 (d, 7.0, 2H)	3.20 (d, 7.0, 2H)	3.19 (d, 6.9 2H)
20	5.22 (m)	5.28–5.20 (m)	5.28–5.23 (m)	5.28–5.21 (m)
21	—	—	—	—
22	0.88 (s, 3H)	0.89 (s, 3H)	0.90 (s, 3H)	0.89 (s, 3H)
23	0.85 (s, 3H)	0.86 (s, 3H)	0.87 (s, 3H)	0.86 (s, 3H)
24	0.74 (s, 3H)	0.76 (s, 3H)	0.77 (s, 3H)	0.75 (s, 3H)
25	1.74 (s, 3H)	1.75 (s, 3H)	1.76 (s, 3H)	1.75 (s, 3H)
26	1.70 (s, 3H)	1.71 (s, 3H)	1.72 (s, 3H)	1.71 (s, 3H)
27	1.63 (s, 3H)	1.64 (s, 3H)	1.65 (s, 3H)	1.64 (s, 3H)
28	1.74 (s, 3H)	1.73 (s, 3H)	1.74 (s, 3H)	1.73 (s, 3H)
29	1.68 (s, 3H)	1.66 (s, 3H)	1.67 (s, 3H)	1.66 (s, 3H)

a) O. Ohno, T. Chiba, S. Todoroki. H. Yoshimura, N. Maru, K. Maekawa, H. Imagawa, K. Yamada, A. Wakamiya, K. Suenaga and D. Uemura, *Chem. Commun.,* 2011, **47**, 12453.

b) I. Hayakawa, T. Nakamura, O. Ohno, K. Suenaga and H. Kigoshi, *Org. Biomol. Chem.,* 2015, **13**, 9969.

c) N. Hu, X. Wang, S. Sun, J. Yang and S. Li, *Org. Chem. Front.,* 2024, **11**, 709.

Table S2. Comparison of ^{13}C NMR spectra of natural halichonine B (**2**) by Suenaga–Uemura group, and synthetic halichonine B (**2**) by Hayakawa–Kigoshi, Li, and our groups.

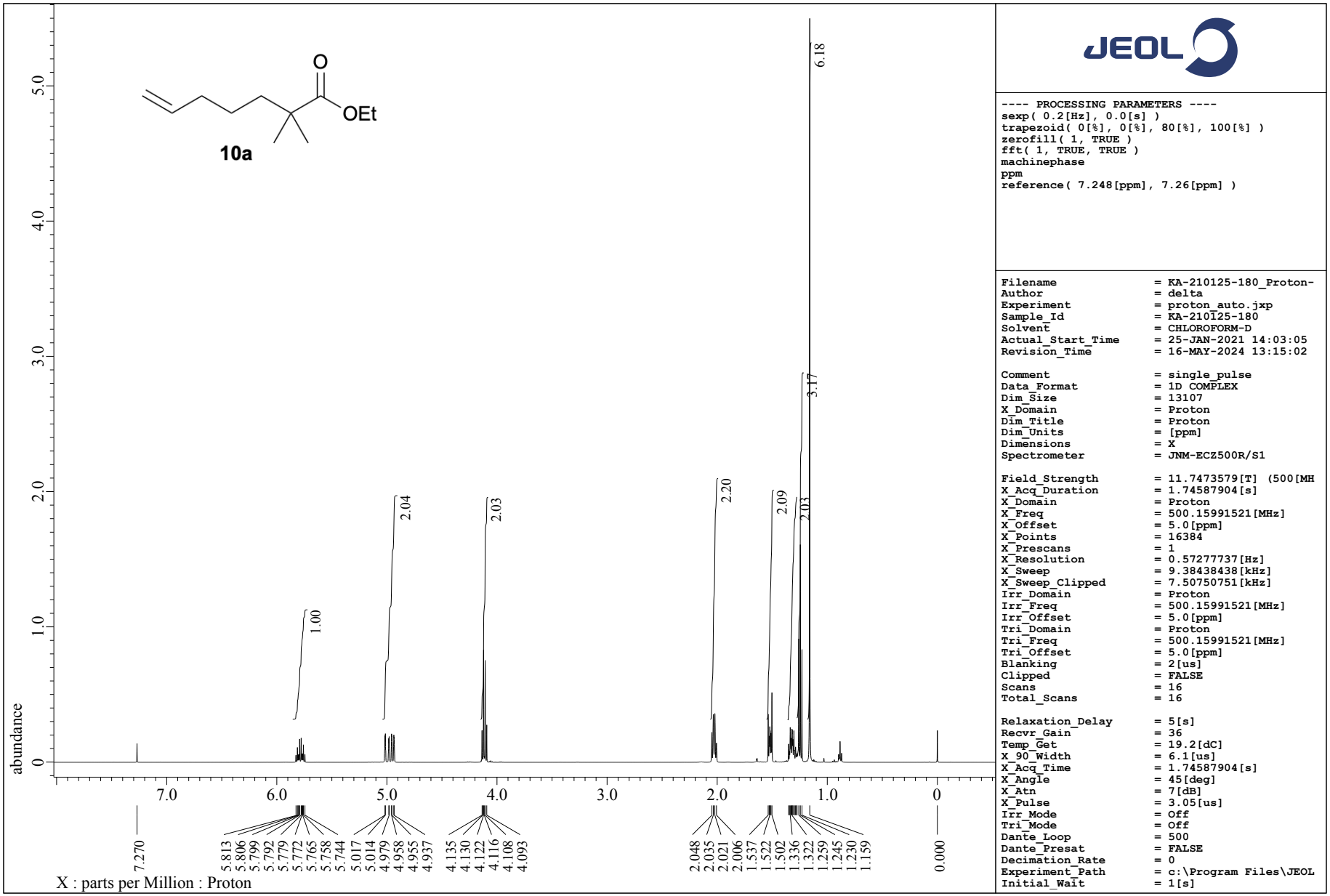
	^{13}C NMR (CD_3OD)			
Carbon No.	Chemical shifts in ppm			
	Suenaga–Uemura (100 MHz)[a]	Hayakawa–Kigoshi (150 MHz)[b]	Li (126 MHz)[c]	This synthesis (125 MHz)
1	39.2	40.6	40.5	40.5
2	18.5	19.9	19.9	19.9
3	42.2	43.5	43.5	43.5
4	32.5	33.9	33.9	33.9
5	50.4	51.7	51.7	51.7
6	23.5	24.8	24.8	24.8
7	121.7	123.1	123.1	123.1
8	135.4	136.0	136.3	135.9
9	51.7	53.1	53.0	53.1
10	36.1	37.4	37.4	37.4
11	53.6	55.0	55.0	54.9

12	51.0	52.4	52.3	52.3
13	121.5	123.0	123.01	123.0
14	134.0	135.2	135.2	135.2
15	53.0	54.5	54.5	54.5
16	24.3	25.8	25.8	25.8
17	26.2	28.5	28.4	28.5
18	48.0	49.9	49.9	50.0
19	45.8	47.6	47.6	47.6
20	119.0	123.0	122.7	123.1
21	137.4	136.8	136.9	136.9
22	21.1	22.4	22.5	22.4
23	32.6	34.0	34.0	34.0
24	12.8	14.2	14.2	14.2
25	21.6	22.9	23.0	22.9
26	24.7	26.1	26.1	26.1
27	16.7	18.0	18.0	18.0
28	24.6	25.9	26.0	26.0
29	16.7	18.1	18.1	18.1

a) O. Ohno, T. Chiba, S. Todoroki. H. Yoshimura, N. Maru, K. Maekawa, H. Imagawa, K. Yamada, A. Wakamiya, K. Suenaga and D. Uemura, *Chem. Commun.,* 2011, **47**, 12453.

b) I. Hayakawa, T. Nakamura, O. Ohno, K. Suenaga and H. Kigoshi, *Org. Biomol. Chem.,* 2015, **13**, 9969.

c) N. Hu, X. Wang, S. Sun, J. Yang and S. Li, *Org. Chem. Front.,* 2024, **11**, 709.

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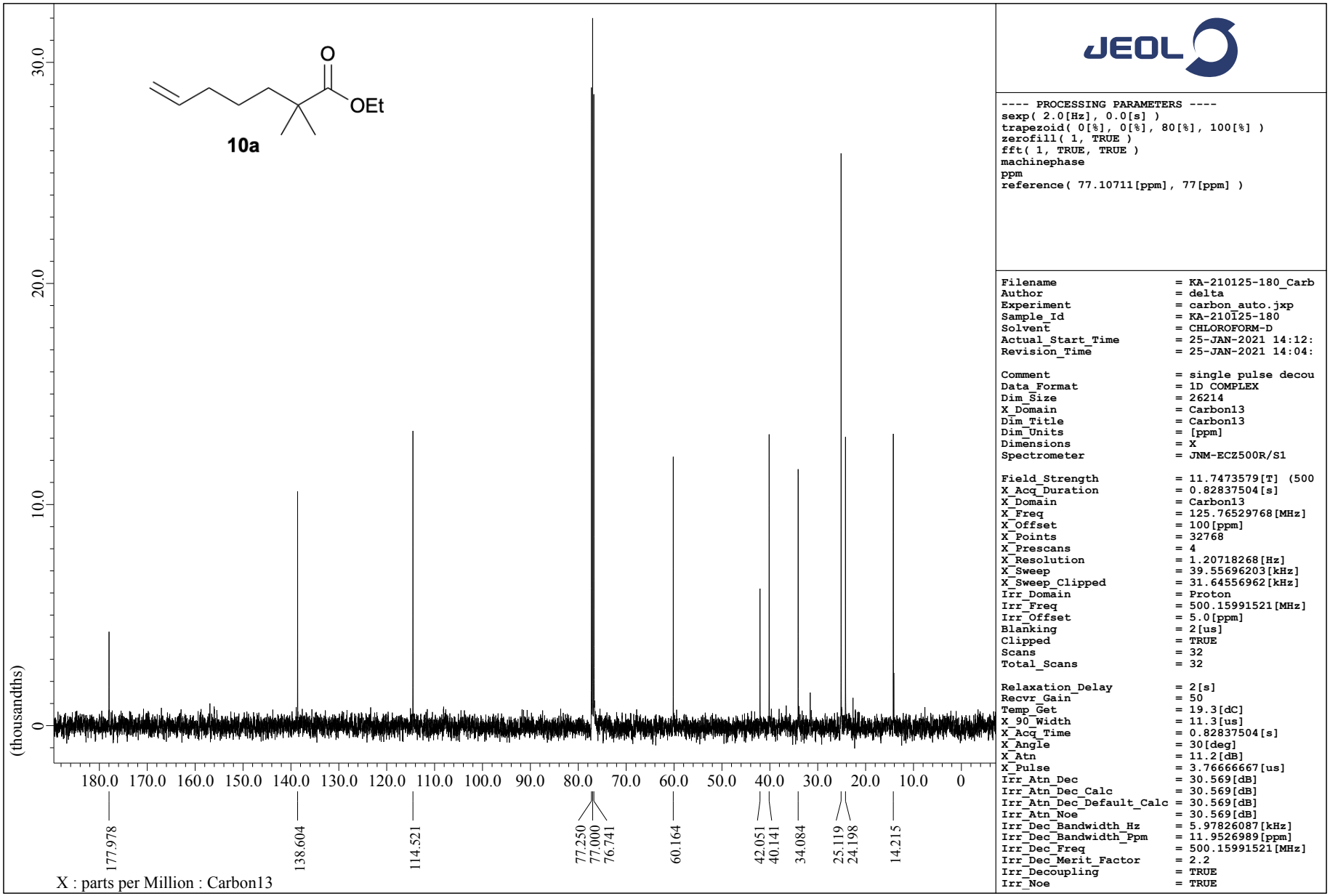
O
OEt
10a
30.0
20.0
10.0
0
(thousandths)
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
177.978
138.604
114.521
77.250
77.000
76.741
60.164
42.051
40.141
34.084
25.119
24.198
14.215
X : parts per Million : Carbon13
JEOL
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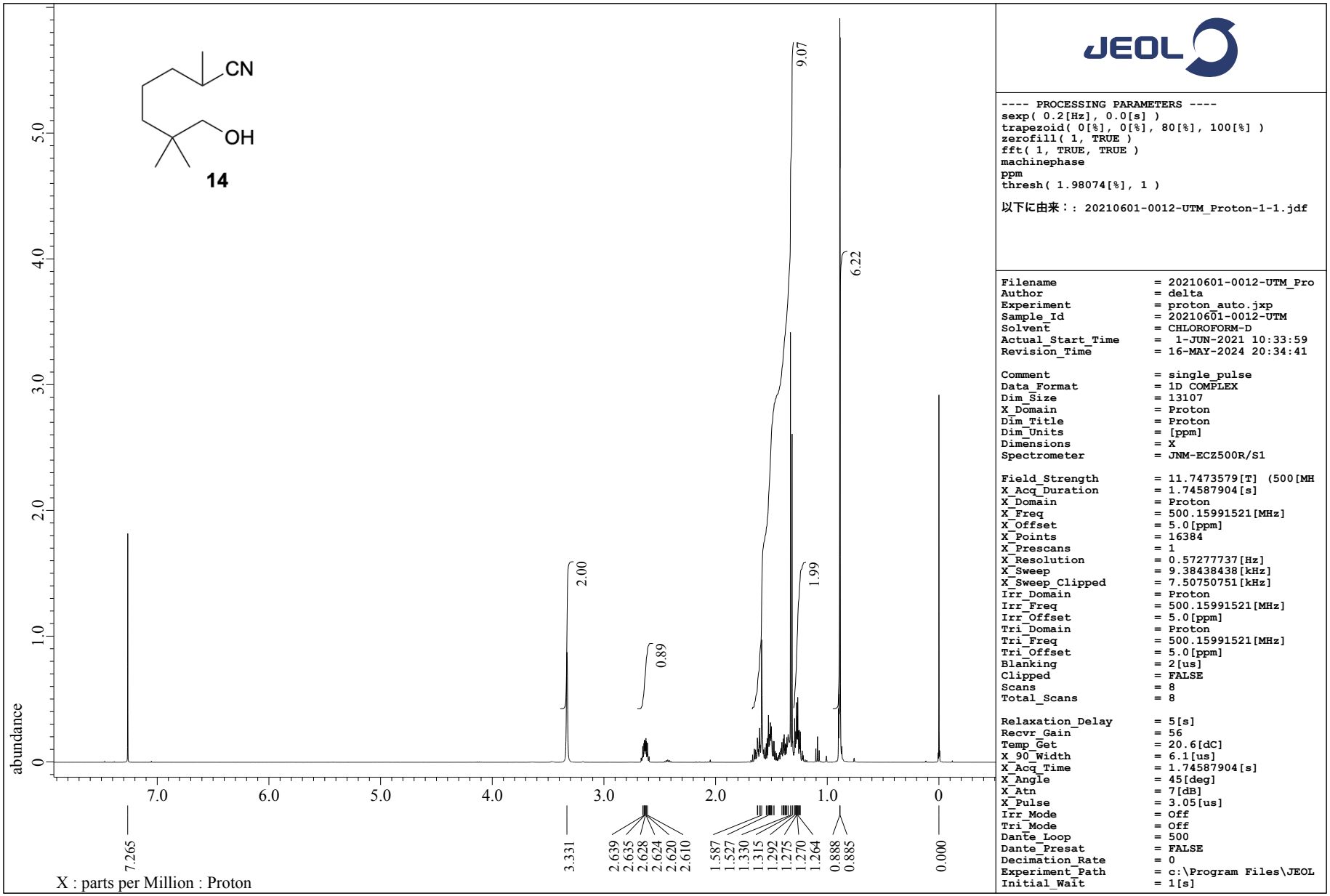
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OH
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X : parts per Million : Proton
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2.635
2.628
2.624
2.620
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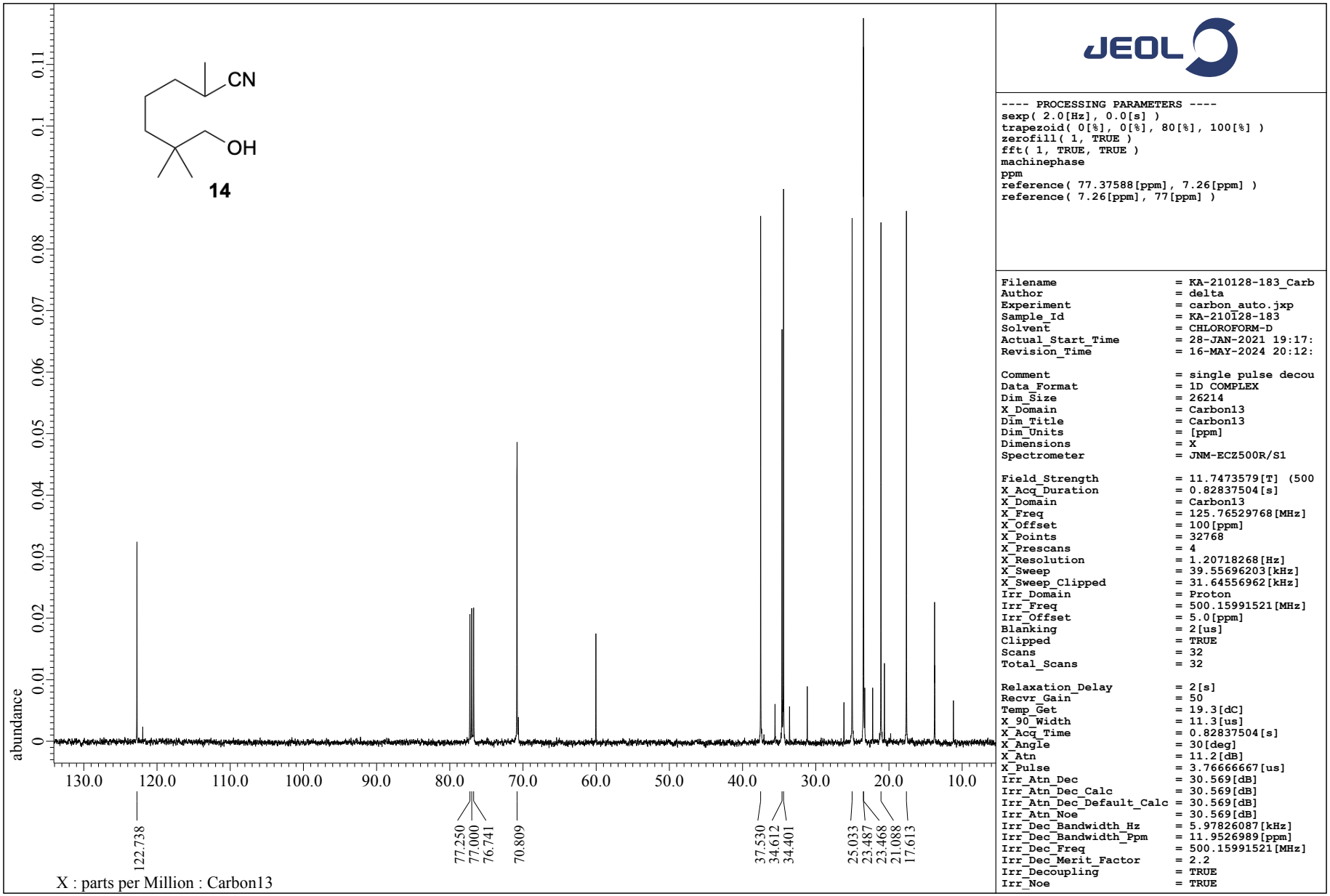


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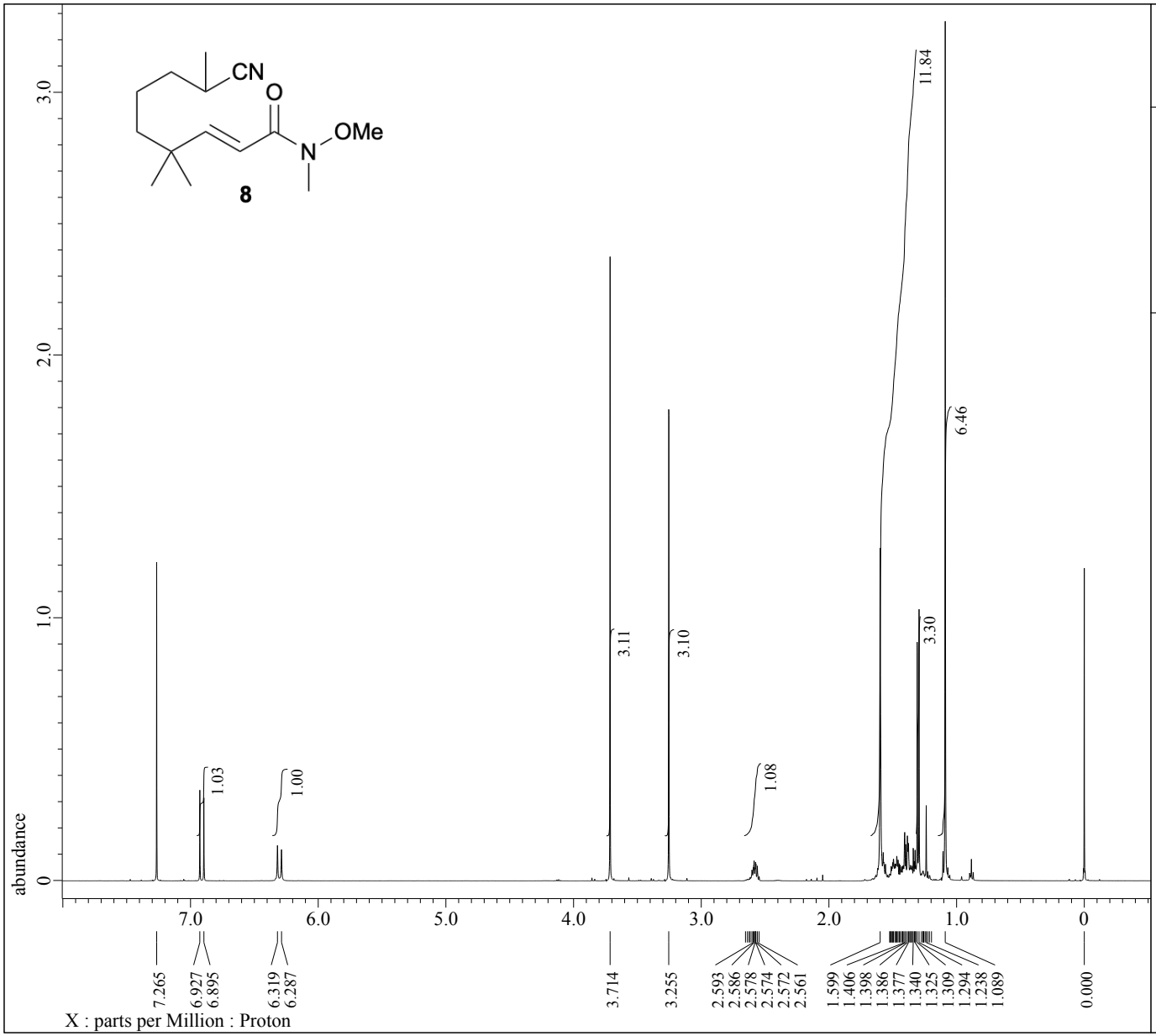


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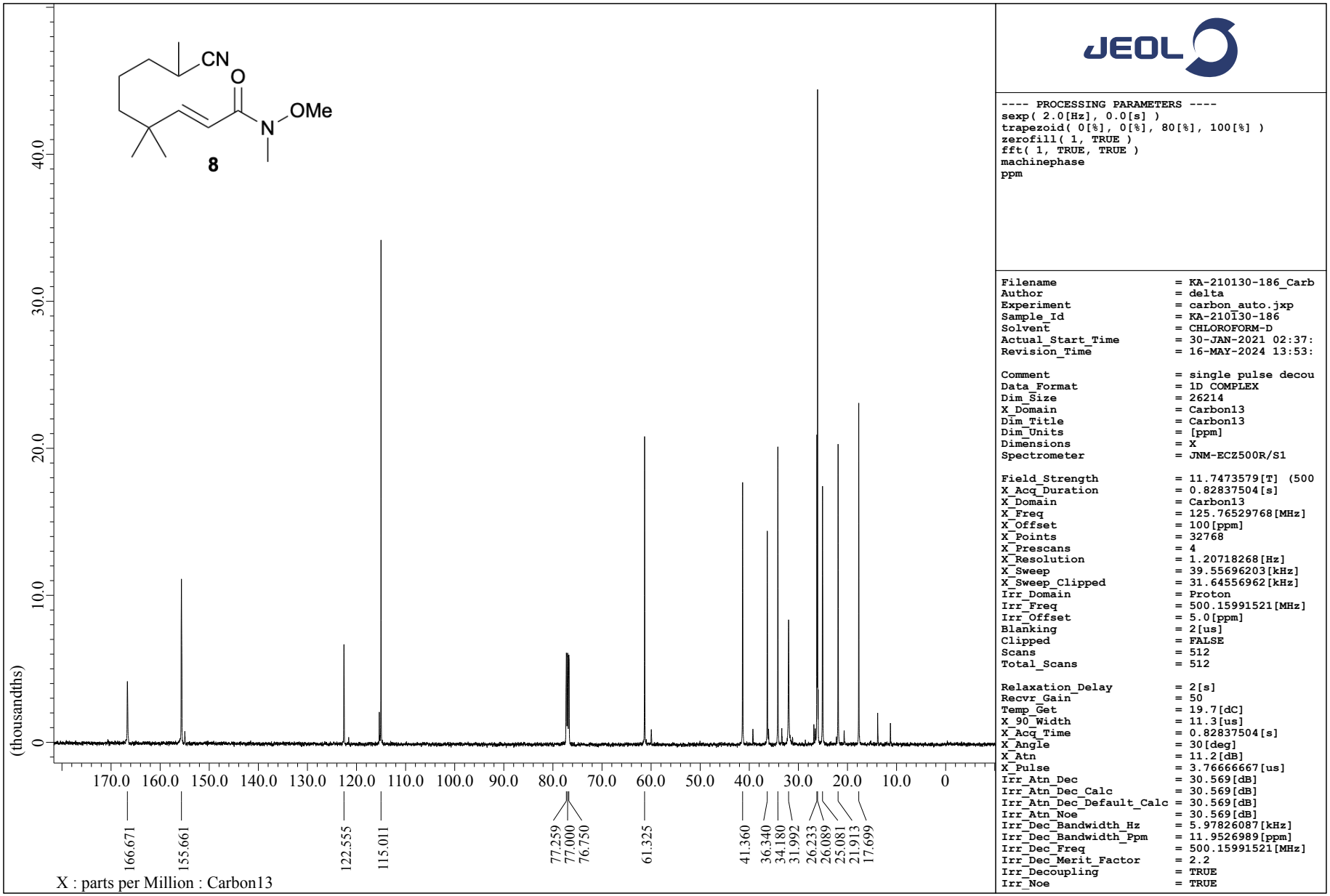
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O
N
OMe
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(thousandths)
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30.0
20.0
10.0
0
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
166.671
155.661
122.555
115.011
77.259
77.000
76.750
61.325
41.360
36.340
34.180
31.992
26.233
26.089
25.081
21.913
17.699
X : parts per Million : Carbon13
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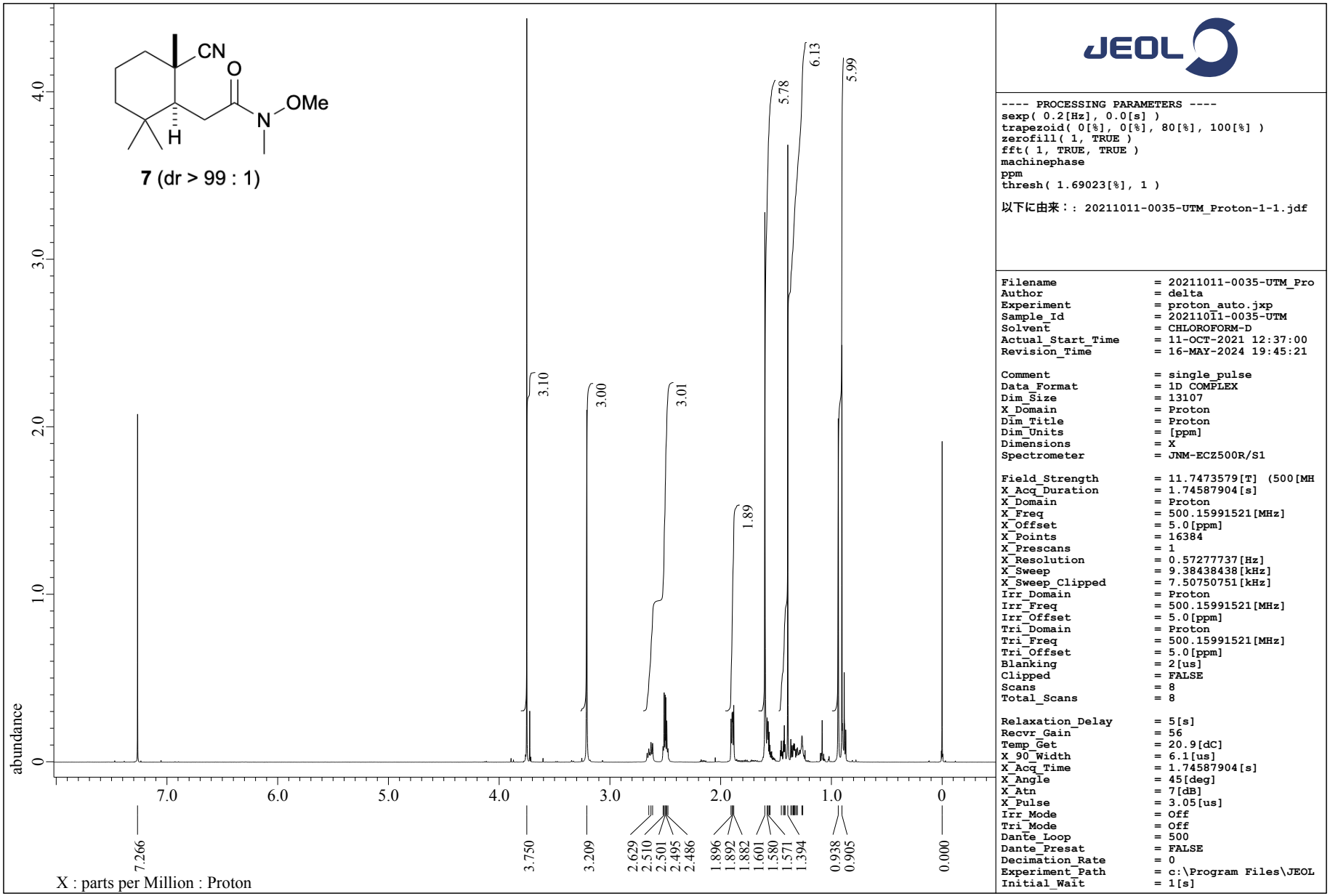
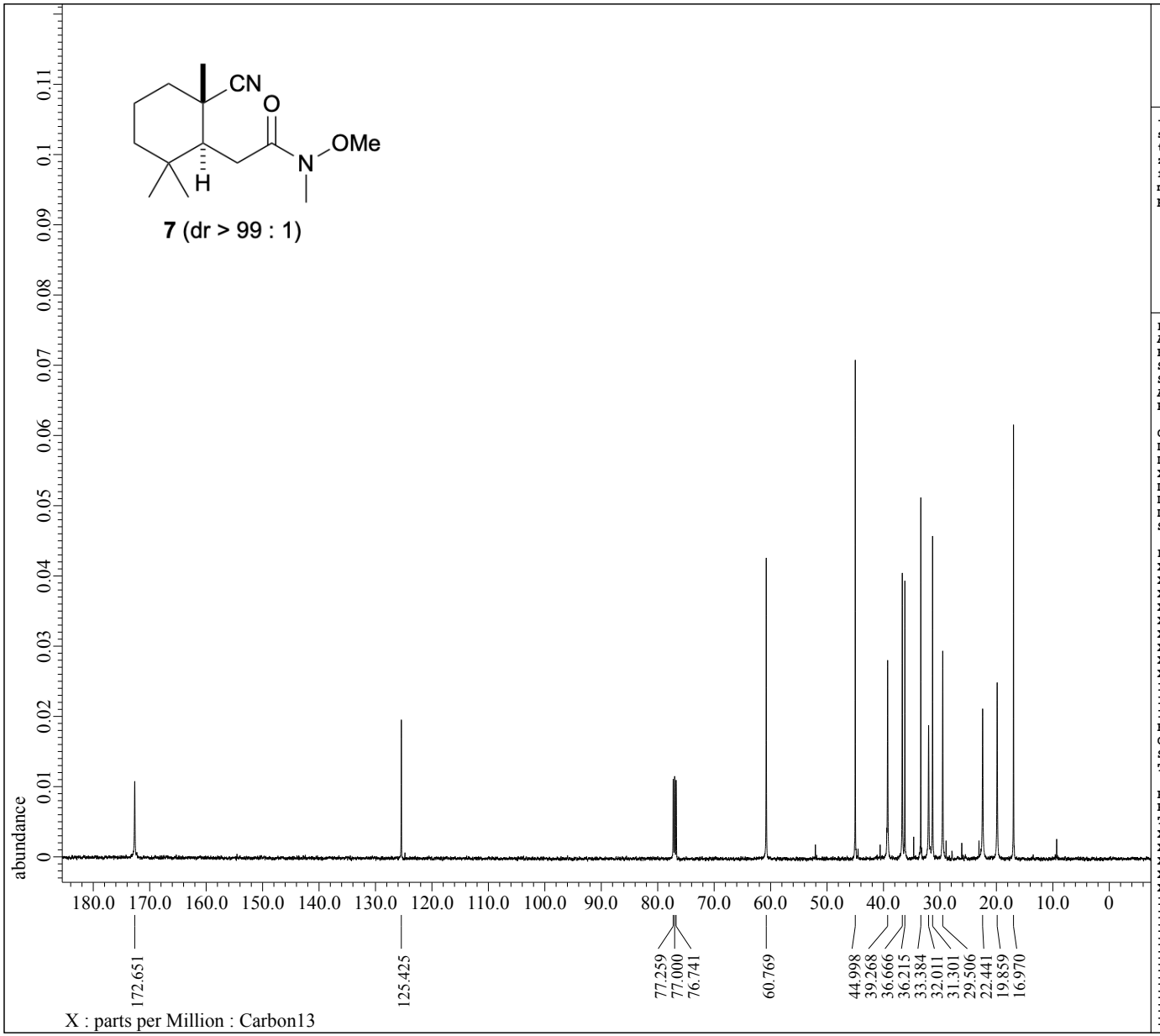
X_Prescans = 4
X_Resolution = 1.20718268[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.7[dC]
X_90_Width = 11.3[us]
X_Acq_Time = 0.82837504[s]
X_Angle = 30[deg]
X_Atn = 11.2[dB]
X_Pulse = 3.76666667[us]
Irr_Atn_Dec = 30.569[dB]
Irr_Atn_Dec_Calc = 30.569[dB]
Irr_Atn_Dec_Default_Calc = 30.569[dB]
Irr_Atn_Noe = 30.569[dB]
Irr_Dec_Bandwidth_Hz = 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.9526989[ppm]
Irr_Dec_Freq = 500.15991521[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 1.69023[%], 1 )

以下に由来：: 20211011-0035-UTM_Proton-1-1.jdf
```

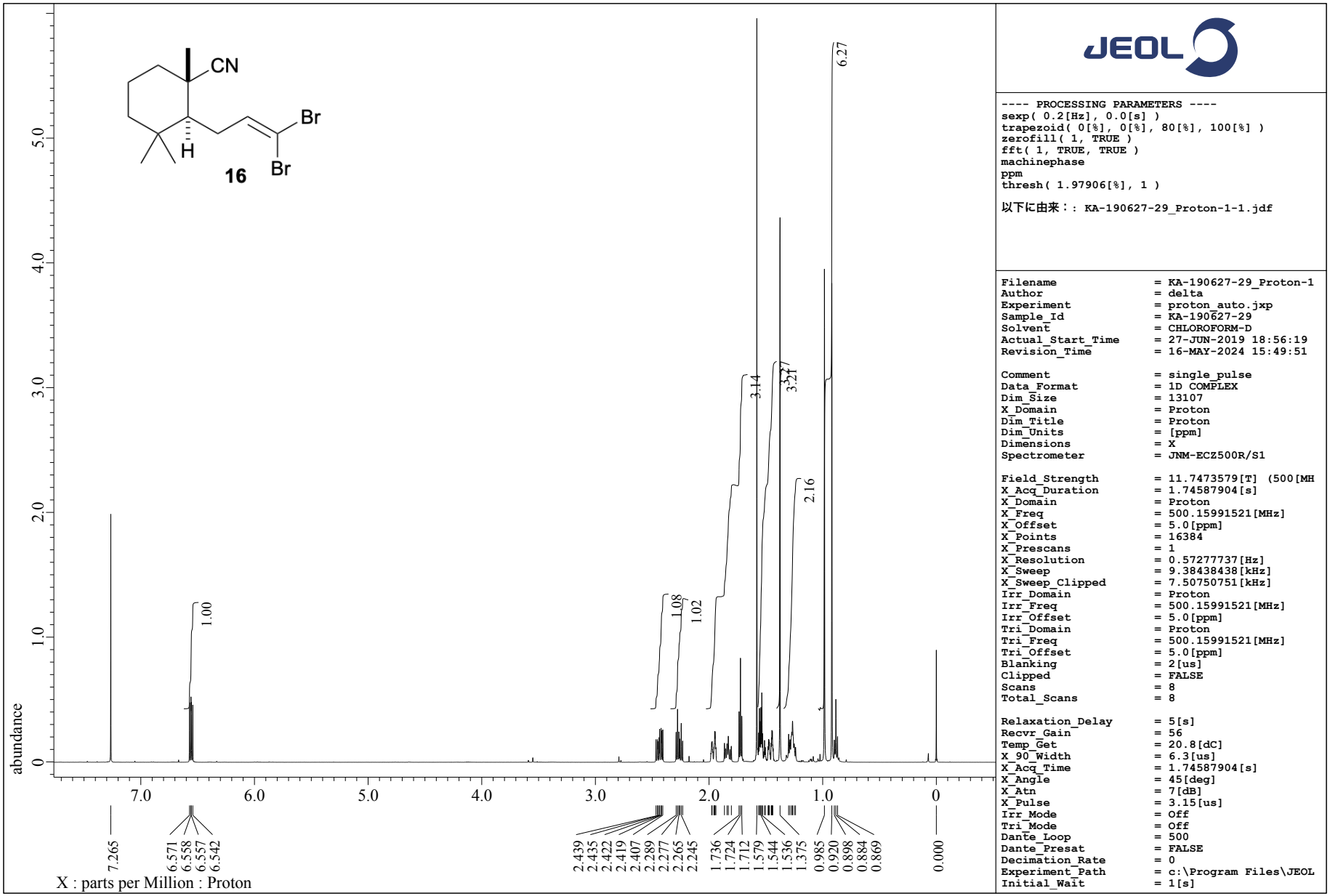
Filename	= 20211011-0035-UTM_Pro
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20211011-0035-UTM
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-OCT-2021 12:37:00
Revision_Time	= 16-MAY-2024 19:45:21
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 20.9[dC]
X_90_Width	= 6.1[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.05[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]



JEOL

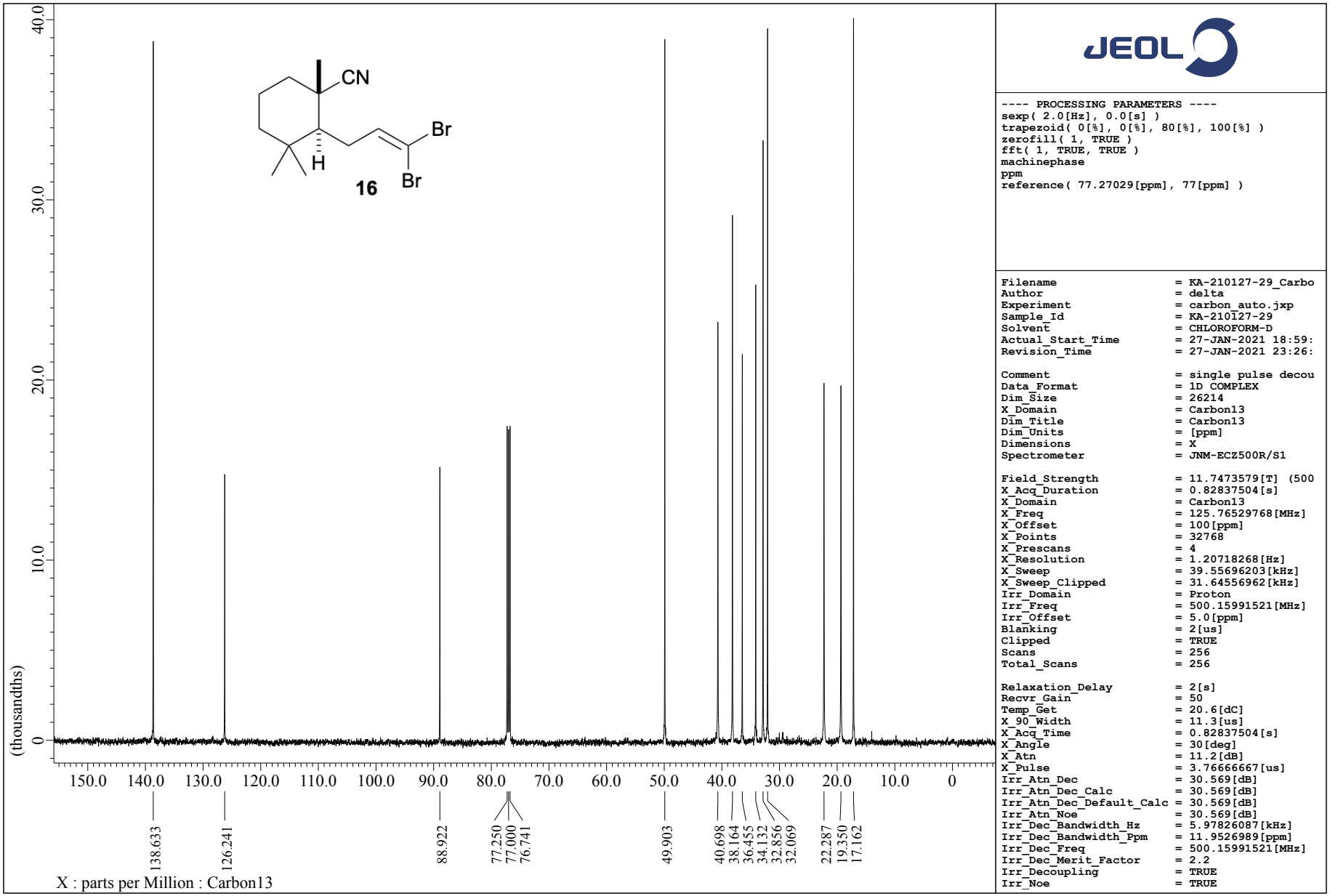
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= KA-210217-5_Carbon
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= KA-210217-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-FEB-2021 19:07:
Revision_Time	= 17-FEB-2021 19:20:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.5[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.76666667[us]
Irr_Atn_Dec	= 30.569[dB]
Irr_Atn_Dec_Calc	= 30.569[dB]
Irr_Atn_Dec_Default_Calc	= 30.569[dB]
Irr_Atn_Noe	= 30.569[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



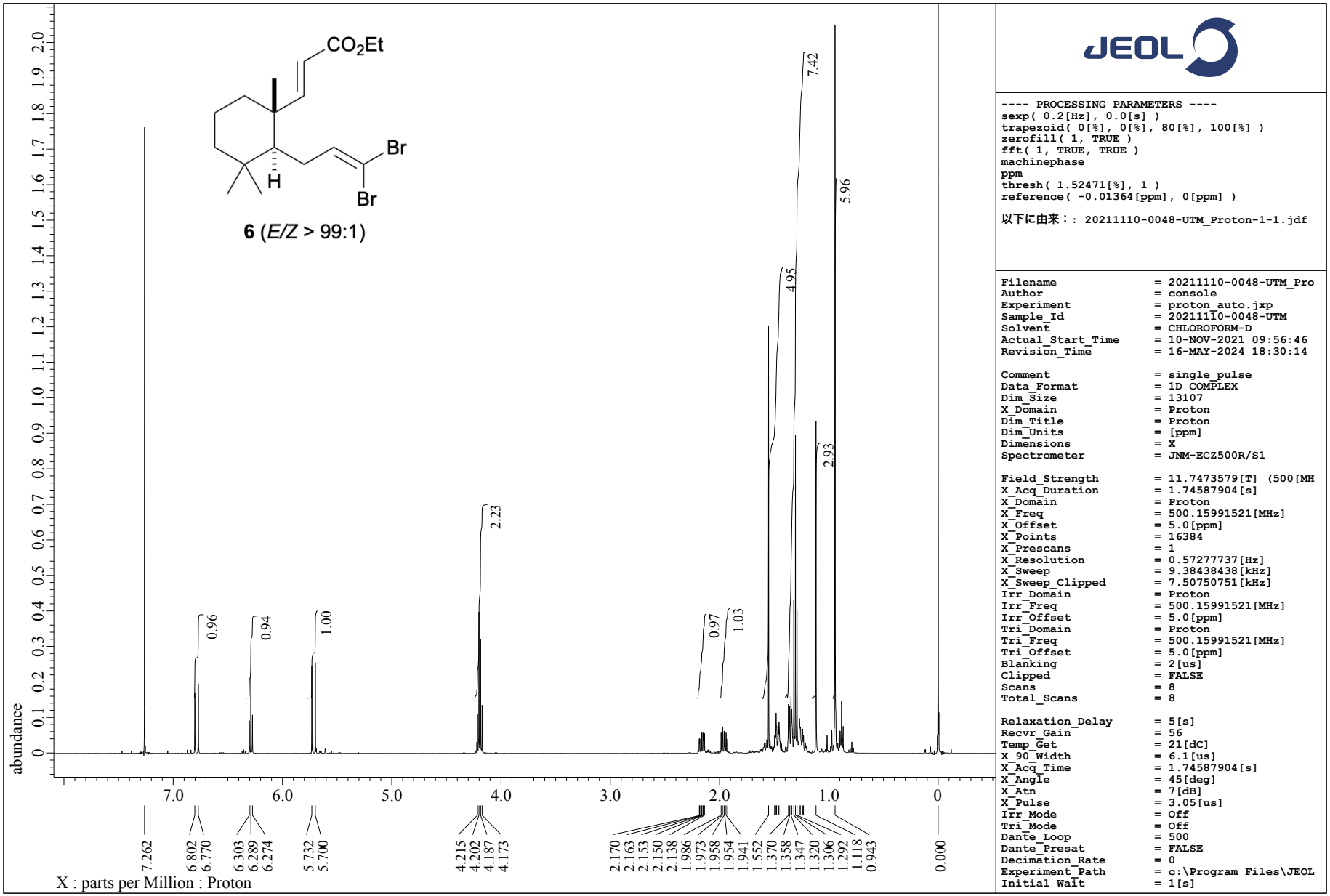

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 1.97906[%], 1 )

以下に由来：: KA-190627-29_Proton-1-1.jdf
```

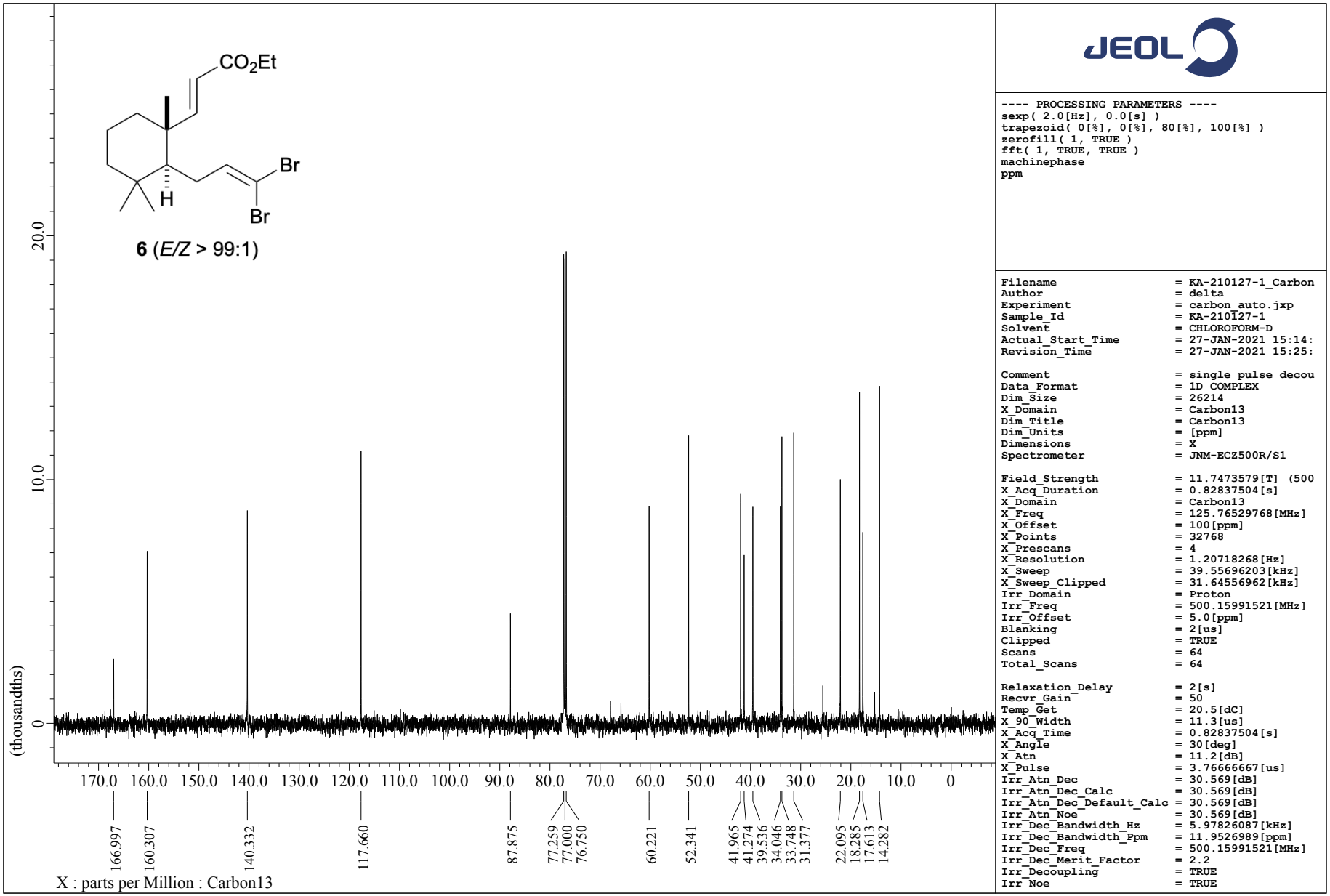
Filename	= KA-190627-29_Proton-1
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= KA-190627-29
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JUN-2019 18:56:19
Revision_Time	= 16-MAY-2024 15:49:51
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[dC]
X_90_Width	= 6.3[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.15[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.27029[ppm], 77[ppm] )
```

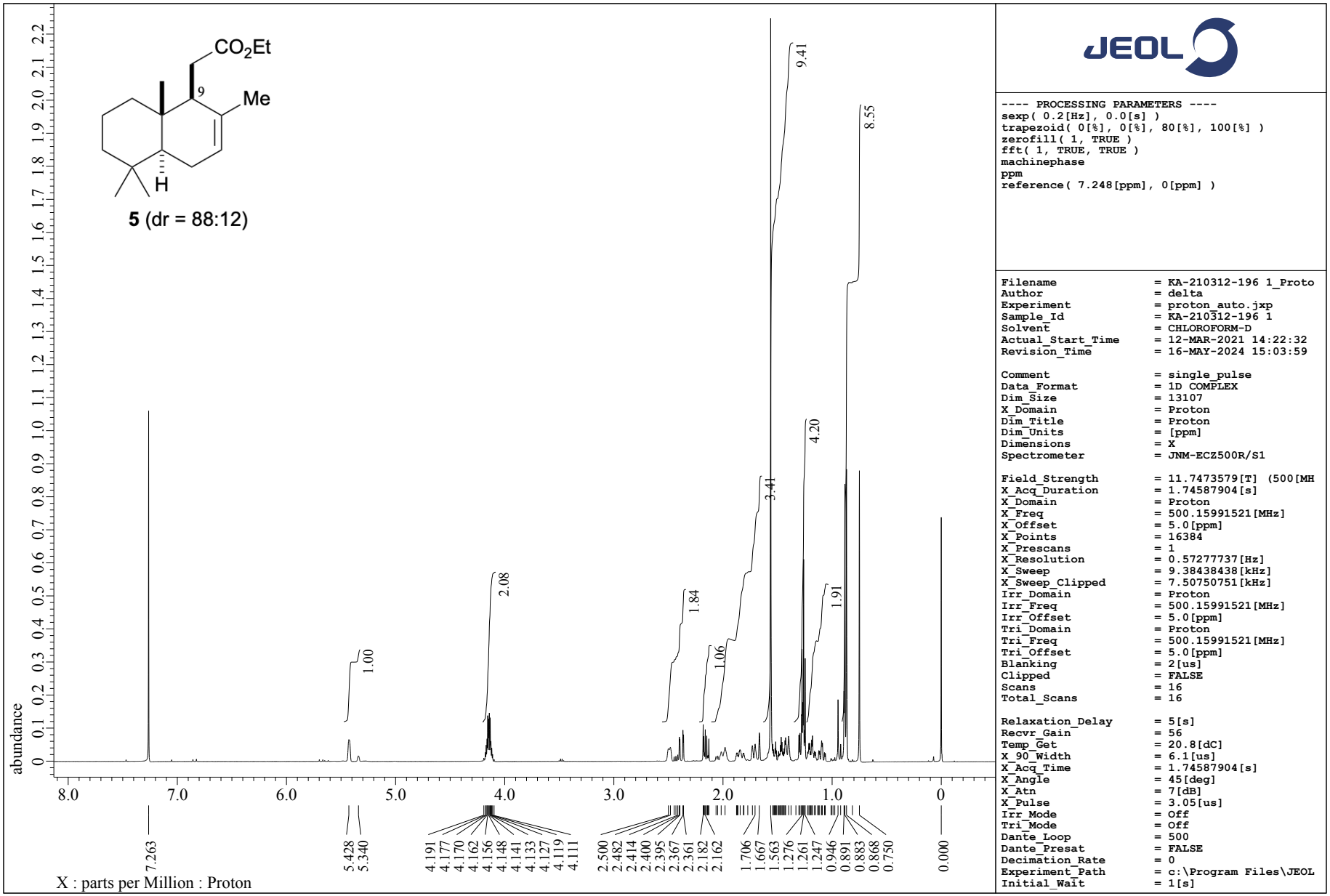
Filename	= KA-210127-29_Carbo
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= KA-210127-29
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JAN-2021 18:59:
Revision_Time	= 27-JAN-2021 23:26:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.6[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.76666667[us]
Irr_Atn_Dec	= 30.569[dB]
Irr_Atn_Dec_Calc	= 30.569[dB]
Irr_Atn_Dec_Default_Calc	= 30.569[dB]
Irr_Atn_Noe	= 30.569[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE


CO2Et
Br
H
Br
6 (E/Z > 99:1)
abundance
X : parts per Million : Proton
7.262
6.802
6.770
6.303
6.289
6.274
5.732
5.700
4.215
4.202
4.187
4.173
2.170
2.163
2.153
2.150
2.138
1.986
1.973
1.958
1.954
1.941
1.552
1.370
1.358
1.347
1.320
1.306
1.292
1.118
0.943
0.000
0.96
0.94
1.00
2.23
0.97
1.03
4.95
7.42
2.93
5.96
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(1.52471[%], 1)
reference(-0.01364[ppm], 0[ppm])
以下に由来：: 20211110-0048-UTM_Proton-1-1.jdf
Filename = 20211110-0048-UTM_Pro
Author = console
Experiment = proton_auto.jxp
Sample_Id = 20211110-0048-UTM
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-NOV-2021 09:56:46
Revision_Time = 16-MAY-2024 18:30:14
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.7473579[T] (500[MH
X_Acq_Duration = 1.74587904[s]
X_Domain = Proton
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
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 = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21[dC]
X_90_Width = 6.1[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 7[dB]
X_Pulse = 3.05[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]



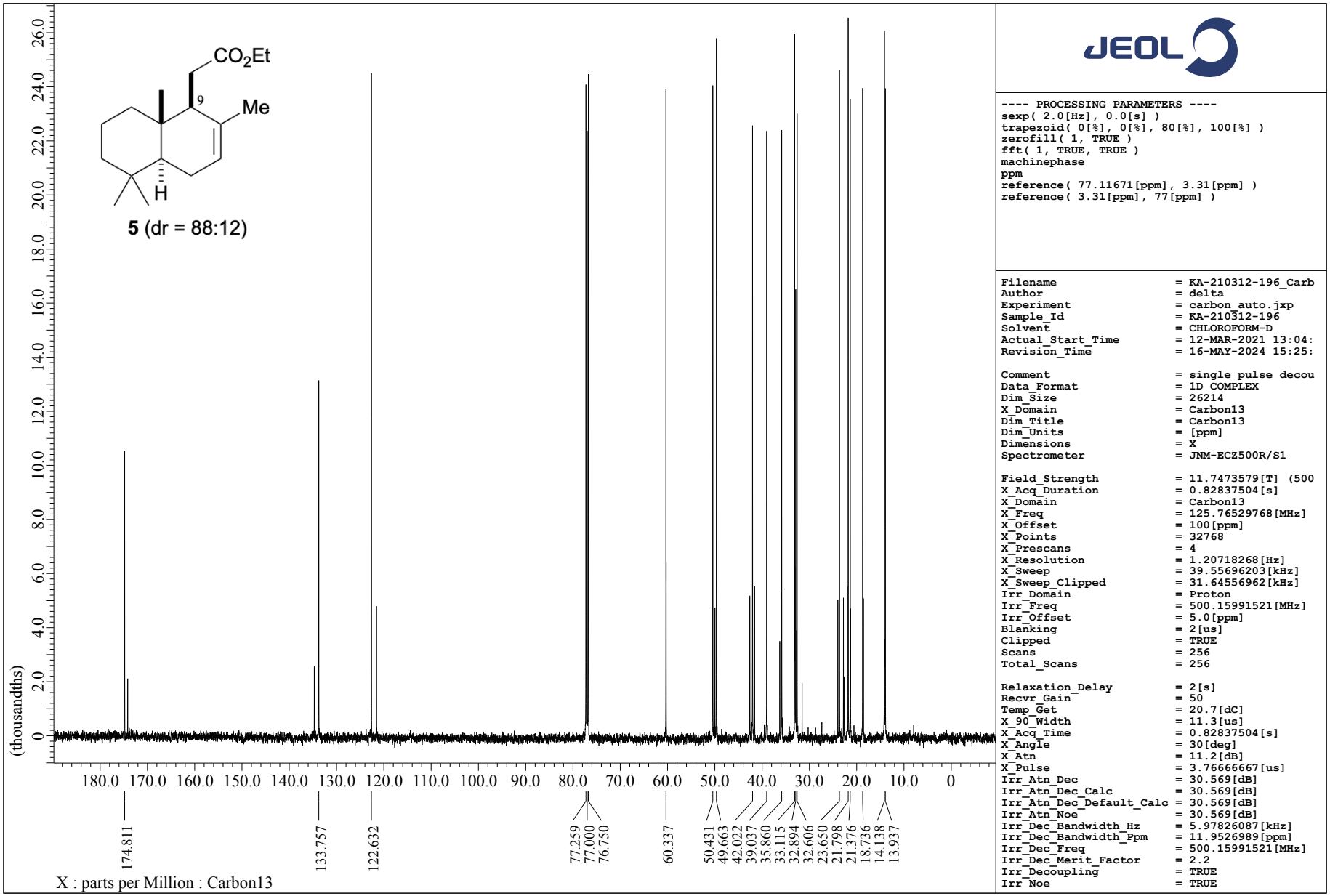

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= KA-210127-1_Carbon
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= KA-210127-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JAN-2021 15:14:
Revision_Time	= 27-JAN-2021 15:25:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.5[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.76666667[us]
Irr_Atn_Dec	= 30.569[dB]
Irr_Atn_Dec_Calc	= 30.569[dB]
Irr_Atn_Dec_Default_Calc	= 30.569[dB]
Irr_Atn_Noe	= 30.569[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



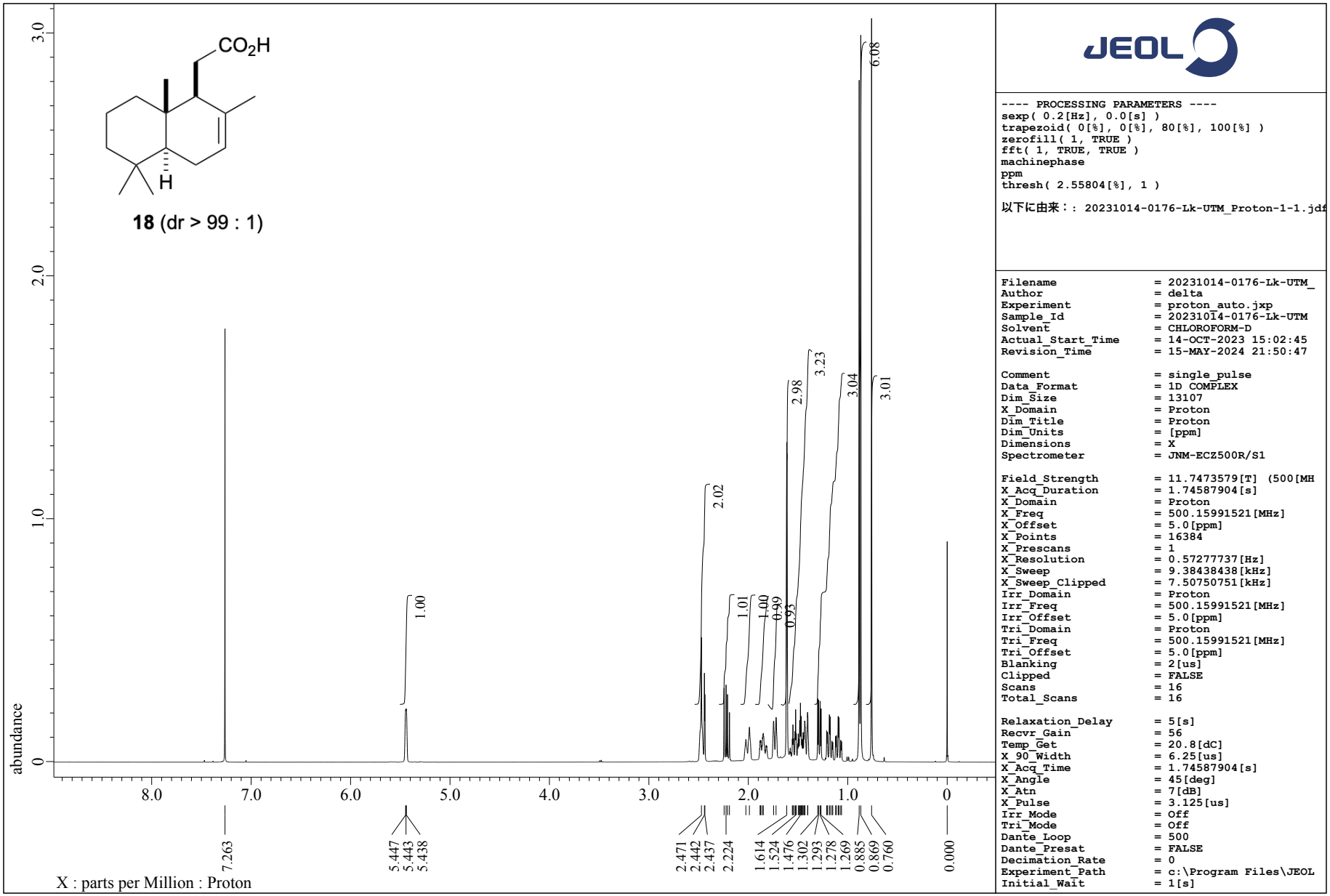

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.248[ppm], 0[ppm] )
```

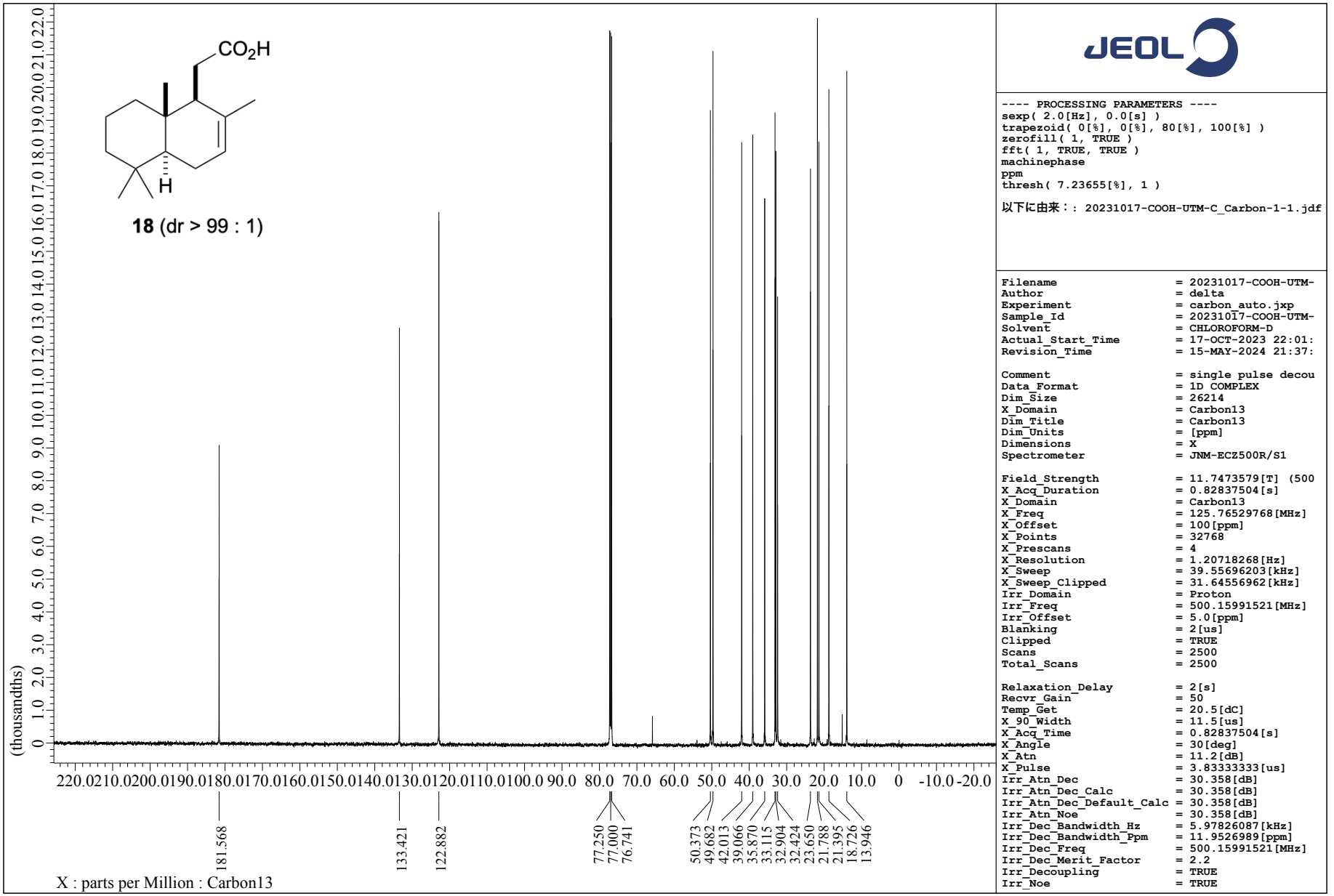
Filename	= KA-210312-196 1_Proto
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= KA-210312-196 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-MAR-2021 14:22:32
Revision_Time	= 16-MAY-2024 15:03:59
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[dC]
X_90_Width	= 6.1[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.05[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.11671[ppm], 3.31[ppm] )
reference( 3.31[ppm], 77[ppm] )
```

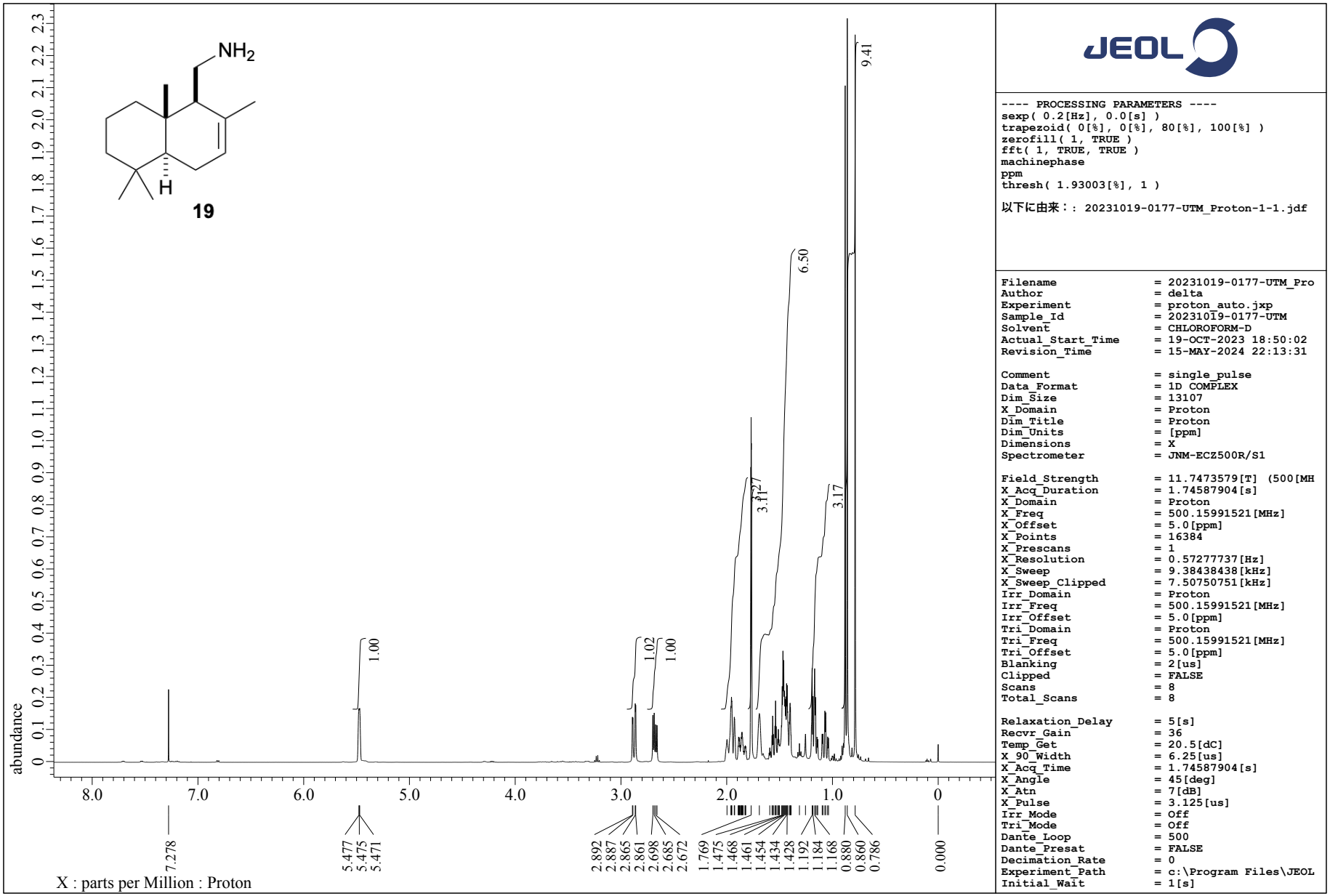
Filename	= KA-210312-196_Carb
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= KA-210312-196
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-MAR-2021 13:04:
Revision_Time	= 16-MAY-2024 15:25:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.7[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.76666667[us]
Irr_Atn_Dec	= 30.569[dB]
Irr_Atn_Dec_Calc	= 30.569[dB]
Irr_Atn_Dec_Default_Calc	= 30.569[dB]
Irr_Atn_Noe	= 30.569[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE


CO2H
H
18 (dr > 99 : 1)
abundance
X : parts per Million : Proton
1.00
2.02
1.01
1.00
0.99
0.93
2.98
3.23
3.04
6.08
3.01
7.263
5.447
5.443
5.438
2.471
2.442
2.437
2.224
1.614
1.524
1.476
1.302
1.293
1.278
1.269
0.885
0.869
0.760
0.000
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(2.55804[%], 1)
以下に由来：: 20231014-0176-Lk-UTM_Proton-1-1.jdf
Filename = 20231014-0176-Lk-UTM_
Author = delta
Experiment = proton_auto.jxp
Sample_Id = 20231014-0176-Lk-UTM
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-OCT-2023 15:02:45
Revision_Time = 15-MAY-2024 21:50:47
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.7473579[T] (500[MH
X_Acq_Duration = 1.74587904[s]
X_Domain = Proton
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
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 = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 20.8[dC]
X_90_Width = 6.25[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 7[dB]
X_Pulse = 3.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]



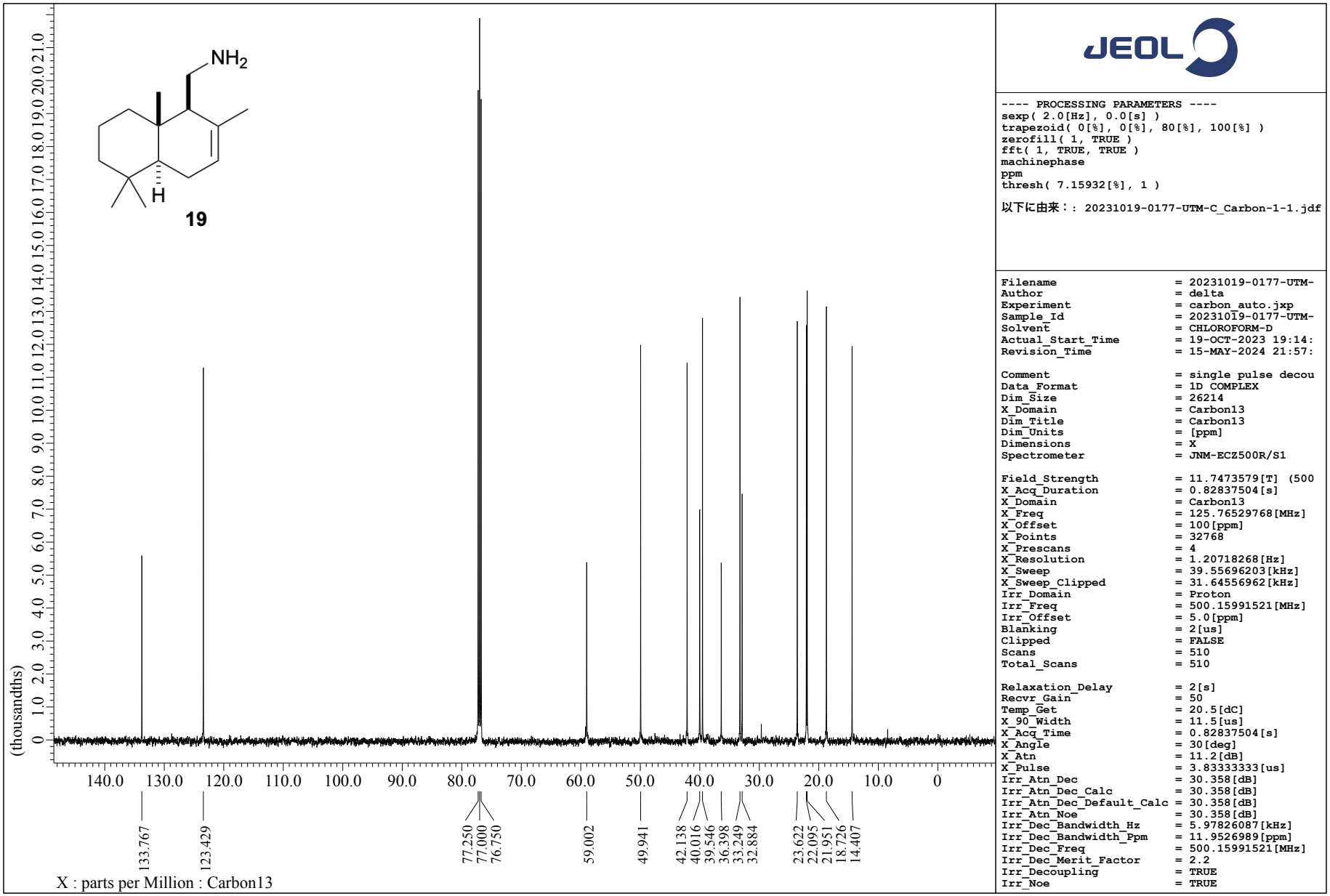

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 7.23655[%], 1 )

以下に由来：: 20231017-COOH-UTM-C_Carbon-1-1.jdf
```

Filename	= 20231017-COOH-UTM-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= 20231017-COOH-UTM-
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-OCT-2023 22:01:
Revision_Time	= 15-MAY-2024 21:37:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 2500
Total_Scans	= 2500
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.5[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.358[dB]
Irr_Atn_Dec_Calc	= 30.358[dB]
Irr_Atn_Dec_Default_Calc	= 30.358[dB]
Irr_Atn_Noe	= 30.358[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



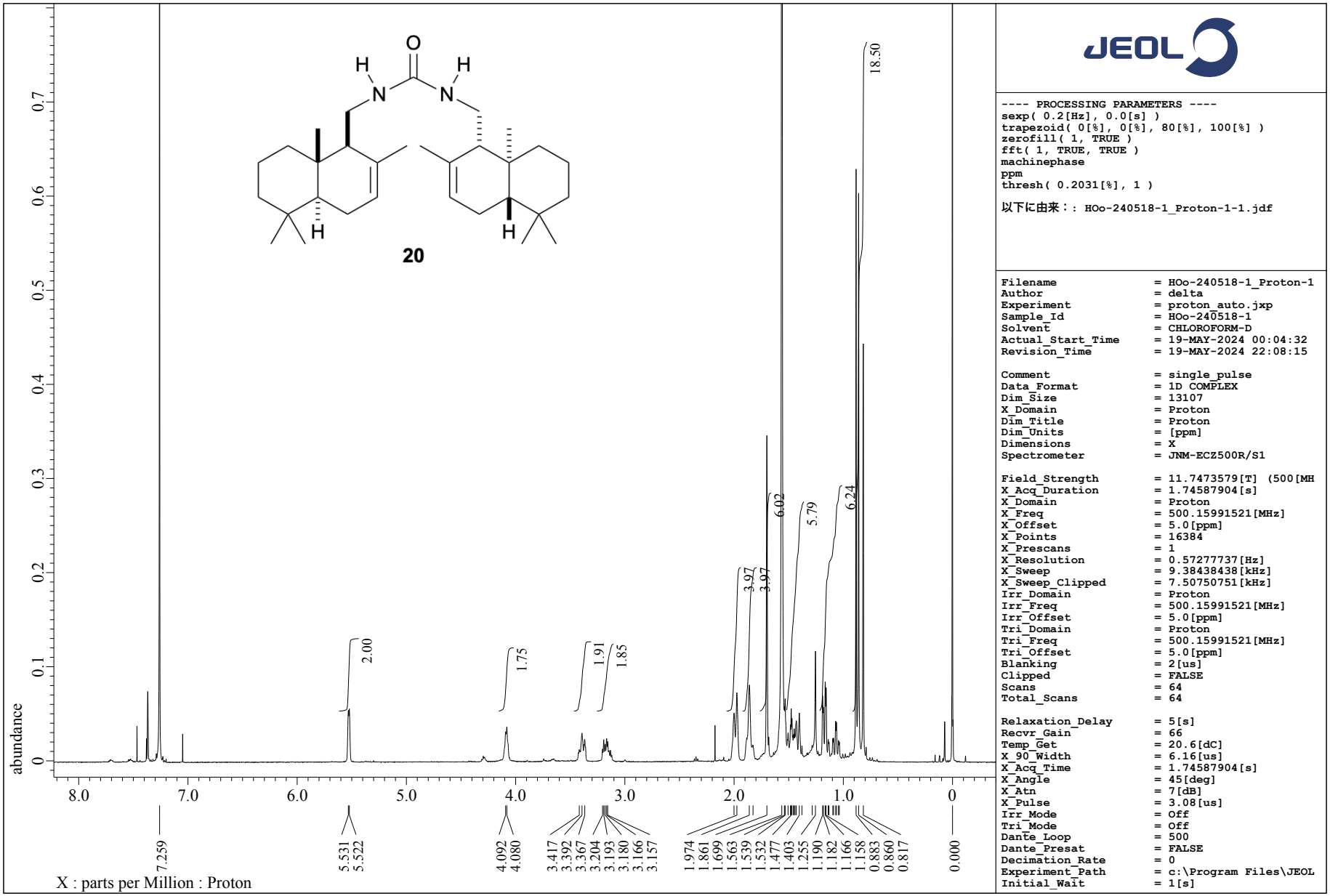

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 1.93003[%], 1 )

以下に由来：: 20231019-0177-UTM_Proton-1-1.jdf
```

Filename	= 20231019-0177-UTM_Pro
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20231019-0177-UTM
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-OCT-2023 18:50:02
Revision_Time	= 15-MAY-2024 22:13:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.5[dC]
X_90_Width	= 6.25[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.125[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]



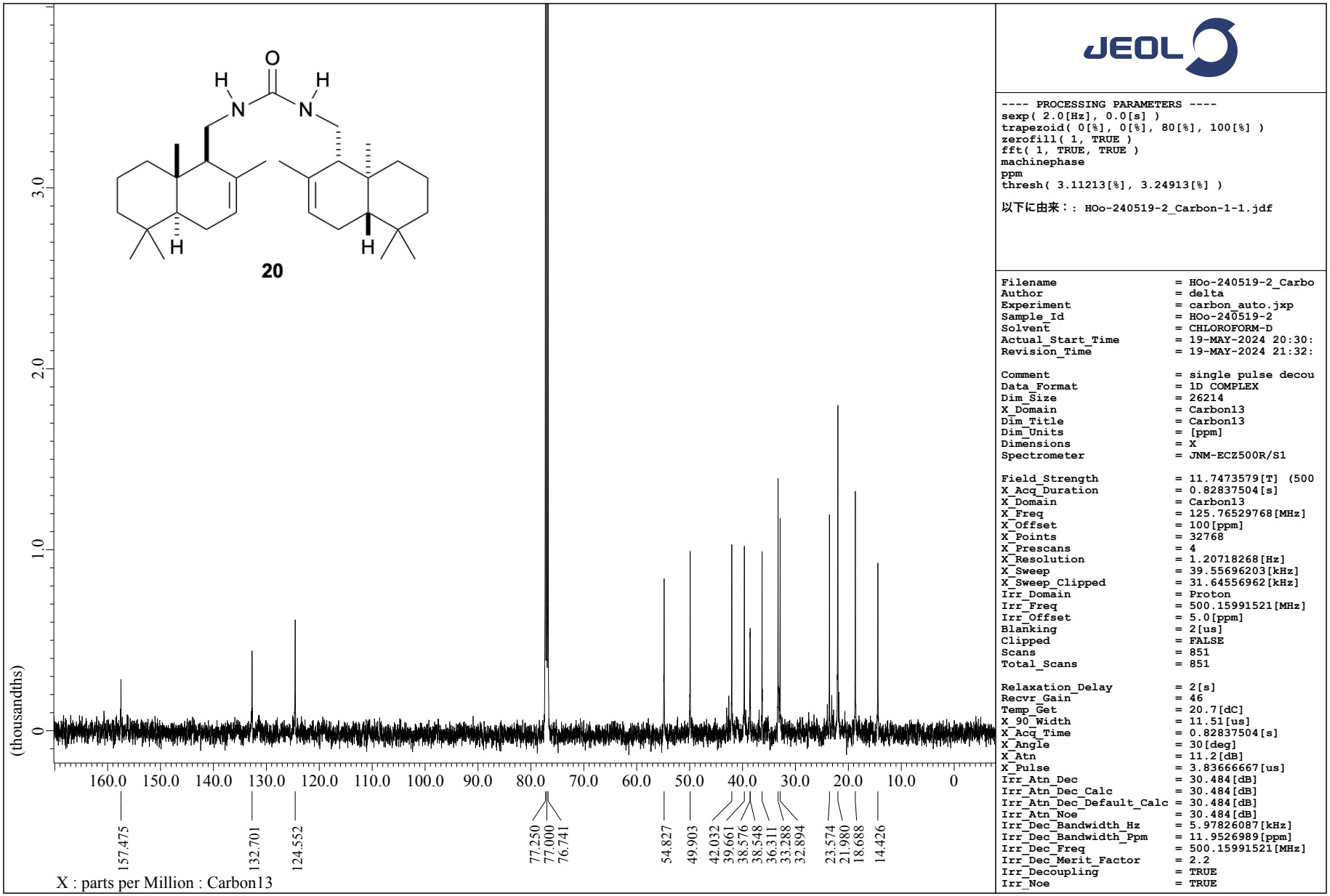

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 7.15932[%], 1 )

以下に由来：: 20231019-0177-UTM-C_Carbon-1-1.jdf
```

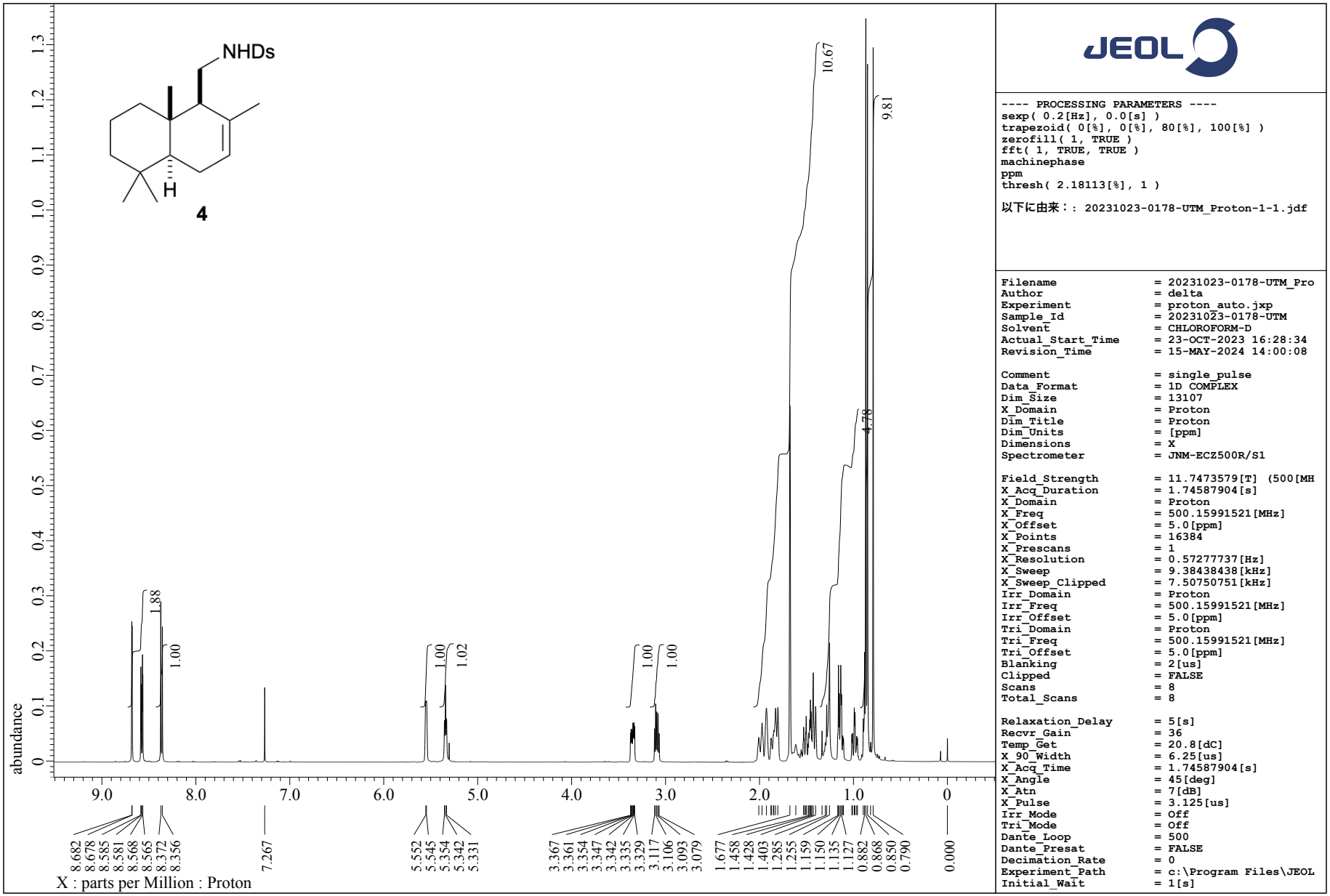
Filename	= 20231019-0177-UTM-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= 20231019-0177-UTM-
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-OCT-2023 19:14:
Revision_Time	= 15-MAY-2024 21:57:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 510
Total_Scans	= 510
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.5[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.358[dB]
Irr_Atn_Dec_Calc	= 30.358[dB]
Irr_Atn_Dec_Default_Calc	= 30.358[dB]
Irr_Atn_Noe	= 30.358[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 0.2031[%], 1 )

以下に由来：: HOo-240518-1_Proton-1-1.jdf
```

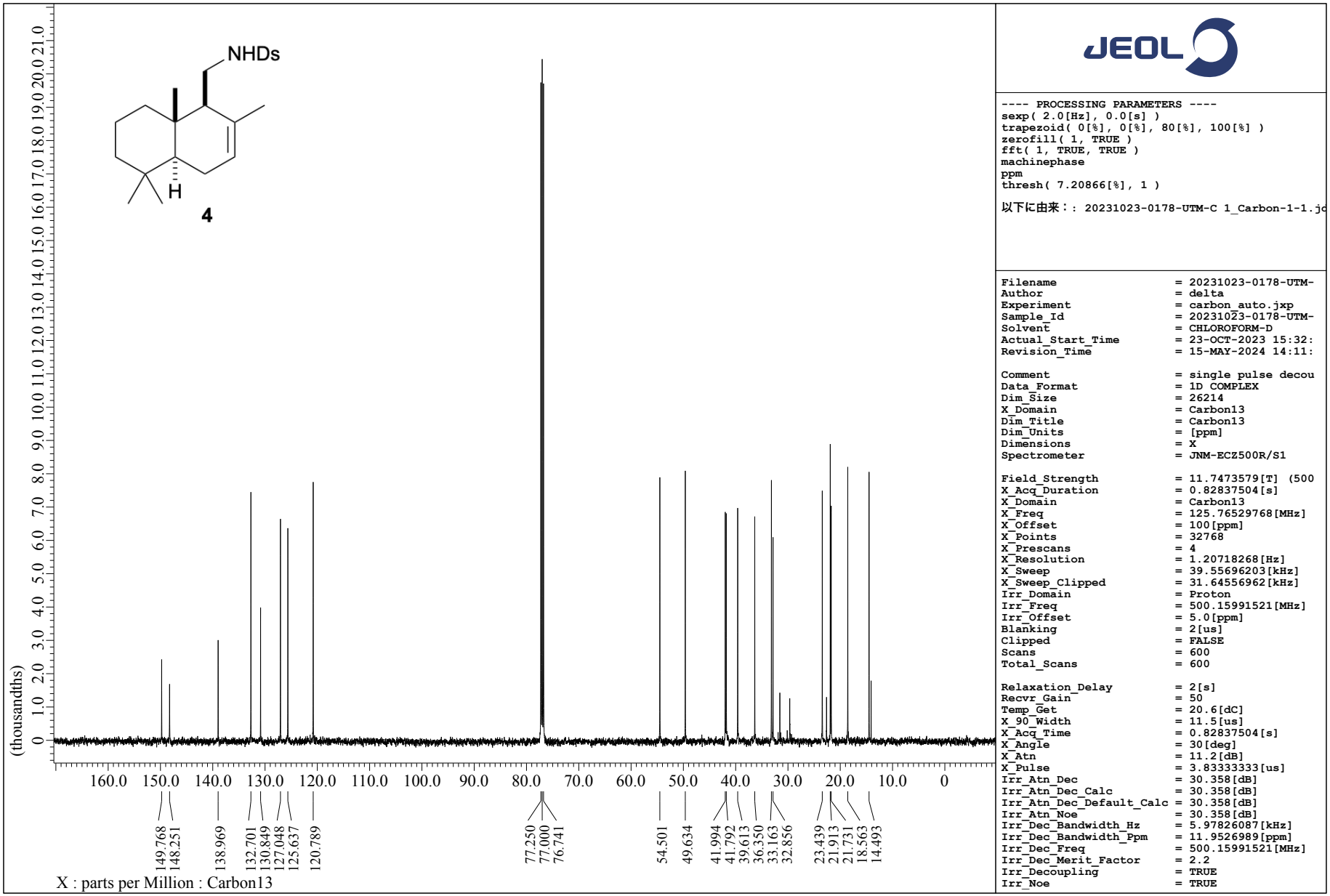
Filename	= HOo-240518-1_Proton-1
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= HOo-240518-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-MAY-2024 00:04:32
Revision_Time	= 19-MAY-2024 22:08:15
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 5[s]
Recvr_Gain	= 66
Temp_Get	= 20.6[dC]
X_90_Width	= 6.16[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.08[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]


20
(thousandths)
3.0
2.0
1.0
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
157.475
132.701
124.552
77.250
77.000
76.741
54.827
49.903
42.032
39.661
38.576
38.548
36.311
33.288
32.894
23.574
21.980
18.688
14.426
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(3.11213[%], 3.24913[%])
以下に由来：: HOo-240519-2_Carbon-1-1.jdf
Filename = HOo-240519-2_Carbo
Author = delta
Experiment = carbon_auto.jxp
Sample_Id = HOo-240519-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-MAY-2024 20:30:
Revision_Time = 19-MAY-2024 21:32:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.7473579[T] (500
X_Acq_Duration = 0.82837504[s]
X_Domain = Carbon13
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.20718268[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 851
Total_Scans = 851
Relaxation_Delay = 2[s]
Recvr_Gain = 46
Temp_Get = 20.7[dC]
X_90_Width = 11.51[us]
X_Acq_Time = 0.82837504[s]
X_Angle = 30[deg]
X_Atn = 11.2[dB]
X_Pulse = 3.83666667[us]
Irr_Atn_Dec = 30.484[dB]
Irr_Atn_Dec_Calc = 30.484[dB]
Irr_Atn_Dec_Default_Calc = 30.484[dB]
Irr_Atn_Noe = 30.484[dB]
Irr_Dec_Bandwidth_Hz = 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.9526989[ppm]
Irr_Dec_Freq = 500.15991521[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE



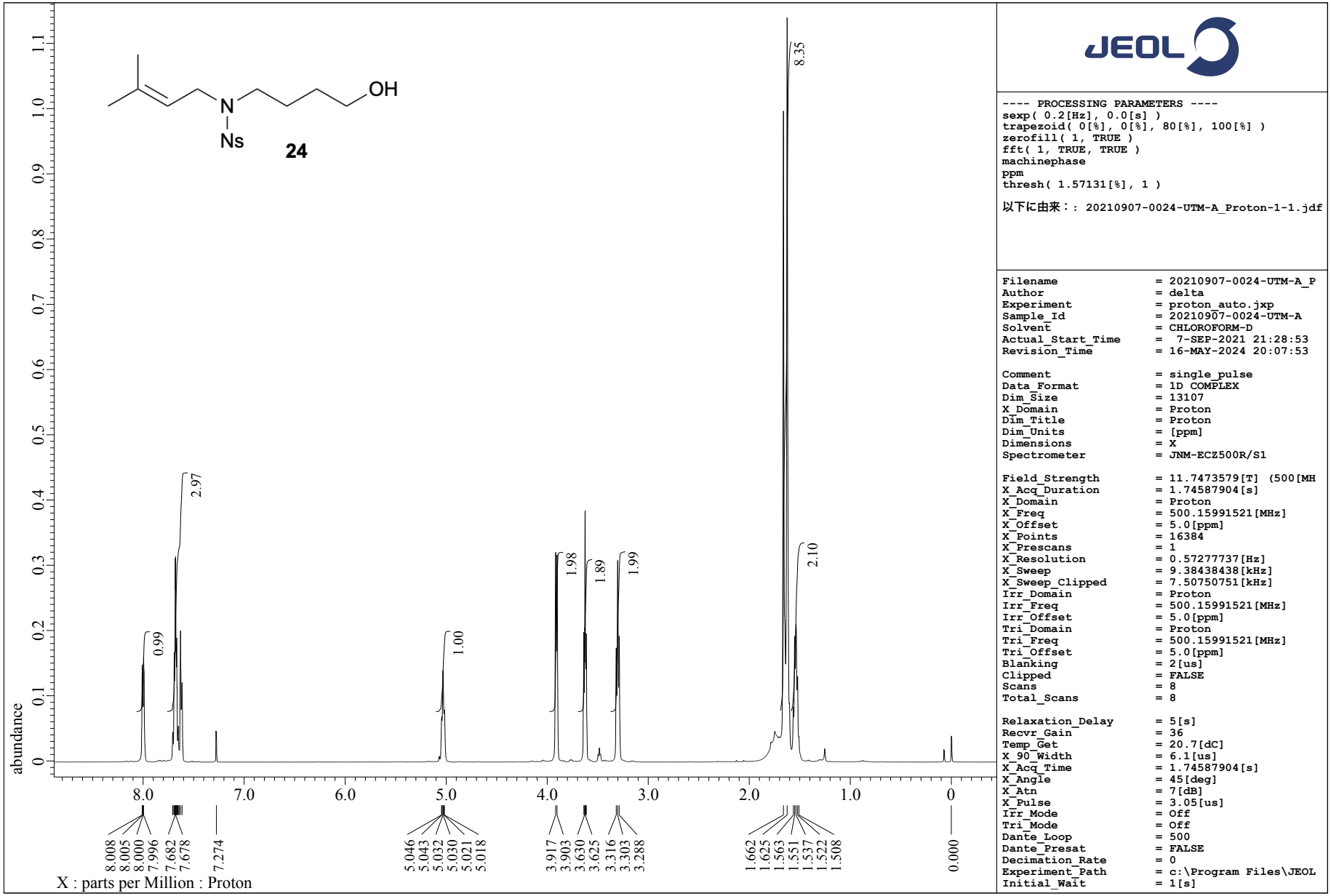

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 2.18113[%], 1 )

以下に由来：: 20231023-0178-UTM_Proton-1-1.jdf
```

Filename	= 20231023-0178-UTM_Pro
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20231023-0178-UTM
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-OCT-2023 16:28:34
Revision_Time	= 15-MAY-2024 14:00:08
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.8[dC]
X_90_Width	= 6.25[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.125[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]



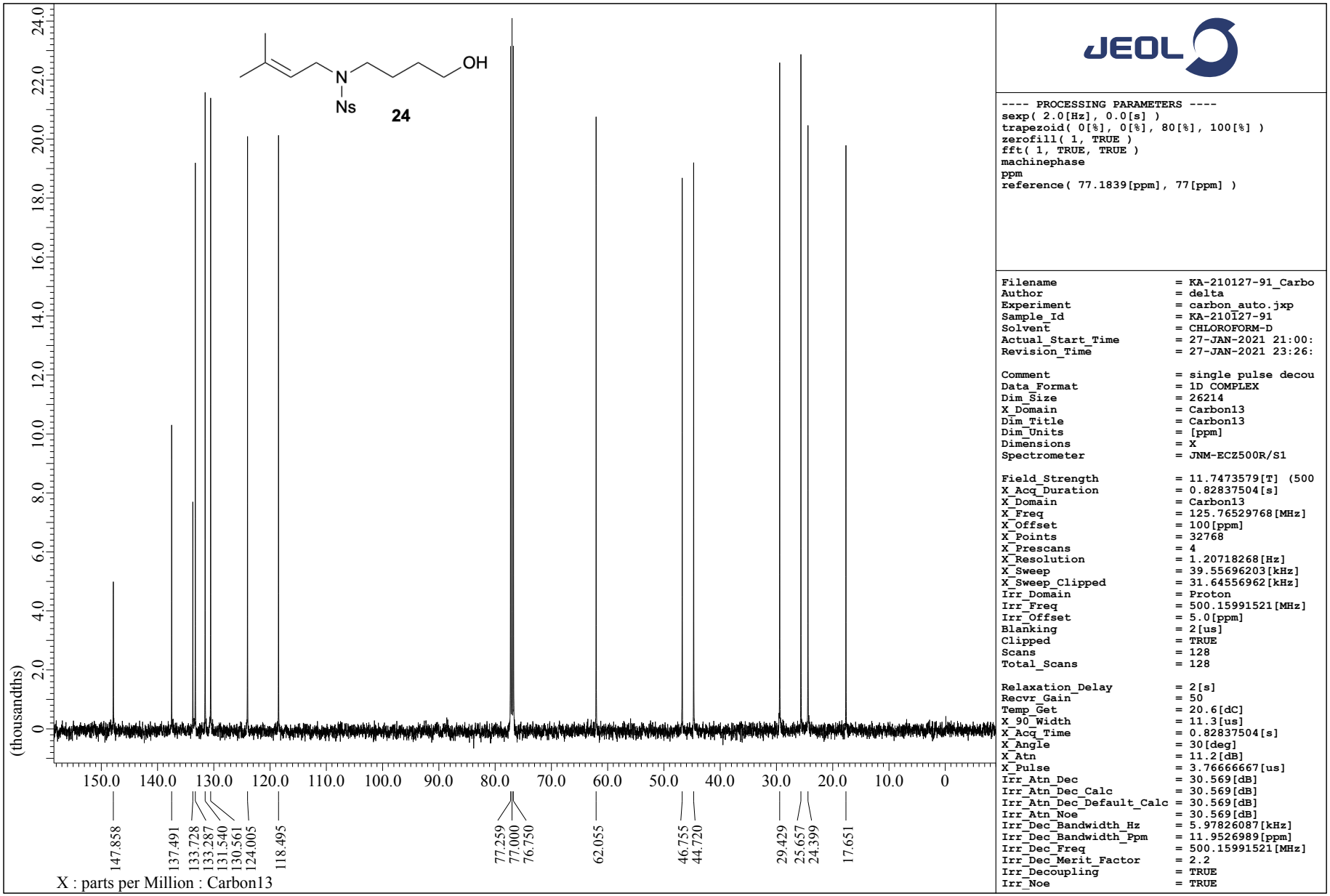

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 7.20866[%], 1 )

以下に由来：: 20231023-0178-UTM-C 1_Carbon-1-1.jd
```

Filename	= 20231023-0178-UTM-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= 20231023-0178-UTM-
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-OCT-2023 15:32:
Revision_Time	= 15-MAY-2024 14:11:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 600
Total_Scans	= 600
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.6[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.358[dB]
Irr_Atn_Dec_Calc	= 30.358[dB]
Irr_Atn_Dec_Default_Calc	= 30.358[dB]
Irr_Atn_Noe	= 30.358[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



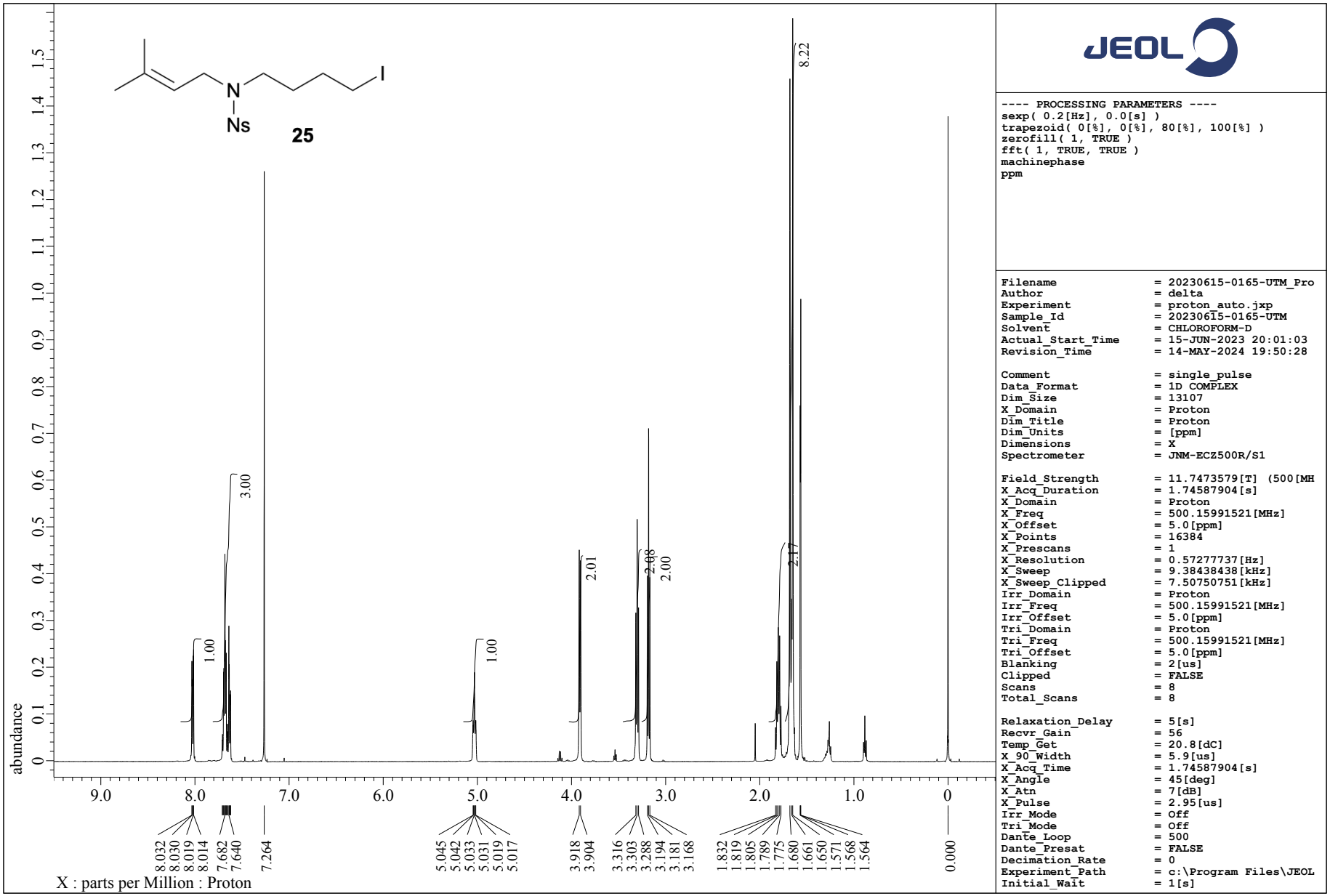

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 1.57131[%], 1 )

以下に由来：: 20210907-0024-UTM-A_Proton-1-1.jdf
```

Filename	= 20210907-0024-UTM-A_P
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20210907-0024-UTM-A
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-SEP-2021 21:28:53
Revision_Time	= 16-MAY-2024 20:07:53
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.7[dC]
X_90_Width	= 6.1[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.05[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]



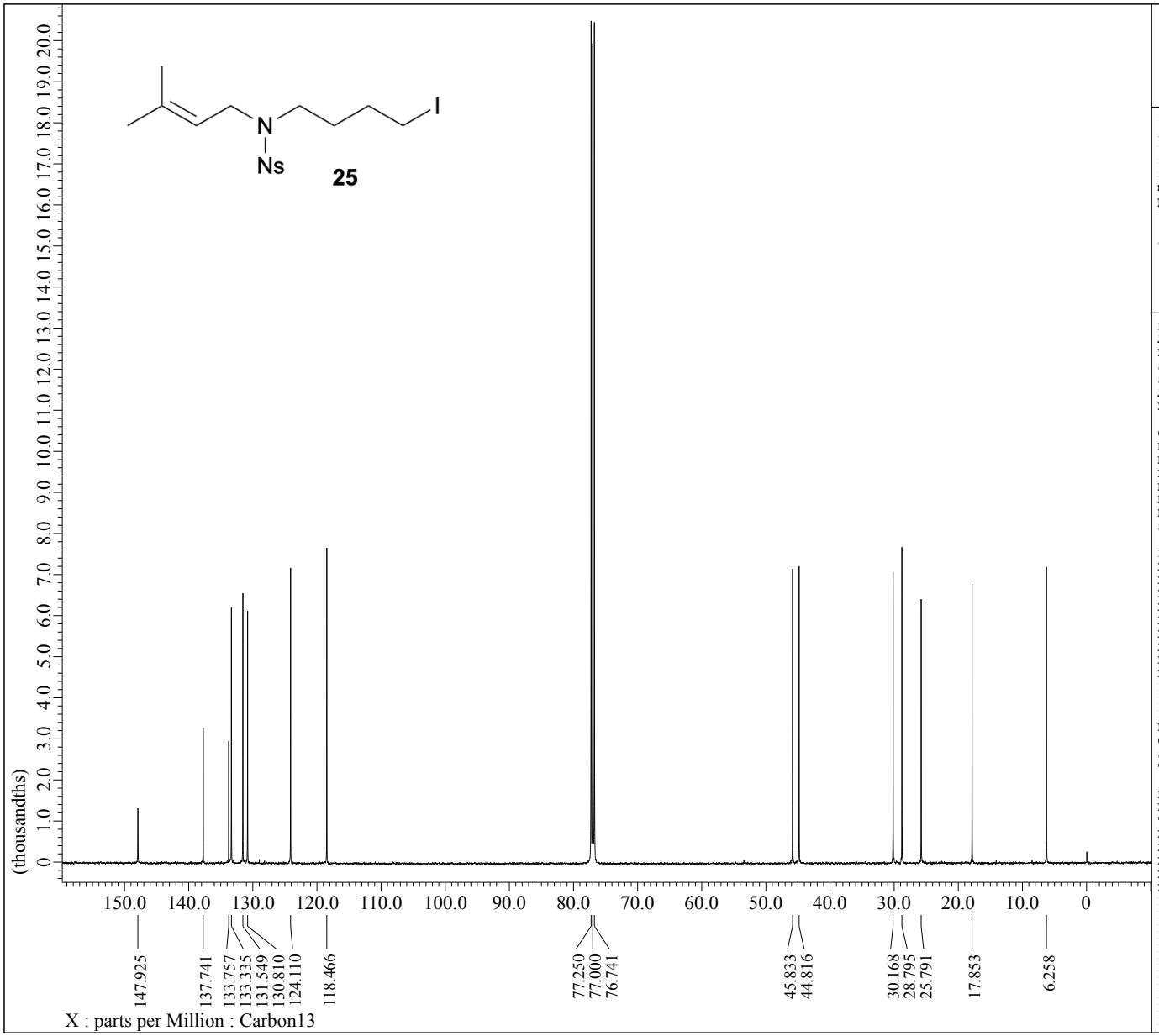

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.1839[ppm], 77[ppm] )
```

Filename	= KA-210127-91_Carbo
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= KA-210127-91
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JAN-2021 21:00:
Revision_Time	= 27-JAN-2021 23:26:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.6[dC]
X_90_Width	= 11.3[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.76666667[us]
Irr_Atn_Dec	= 30.569[dB]
Irr_Atn_Dec_Calc	= 30.569[dB]
Irr_Atn_Dec_Default_Calc	= 30.569[dB]
Irr_Atn_Noe	= 30.569[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



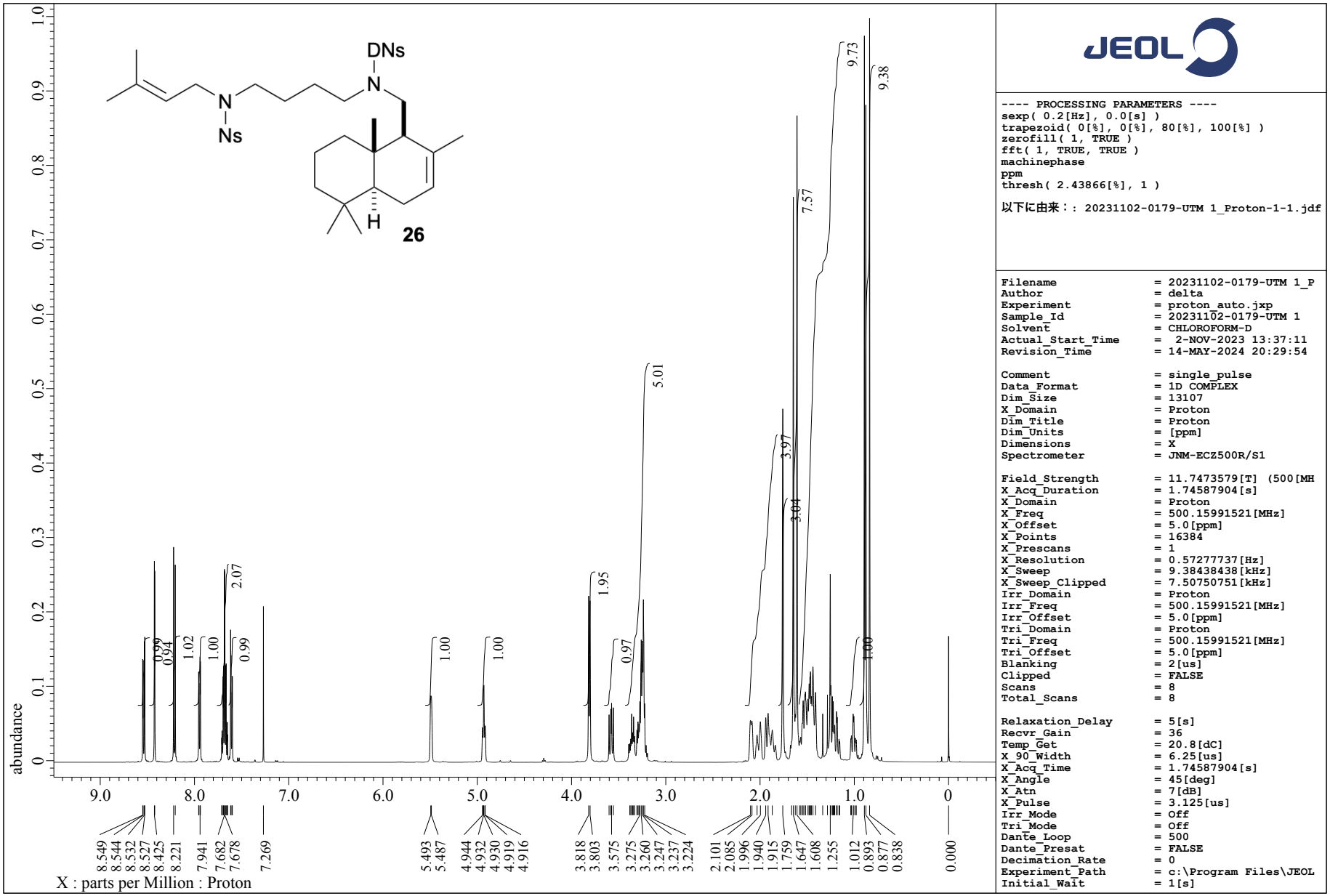

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20230615-0165-UTM_Pro
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20230615-0165-UTM
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JUN-2023 20:01:03
Revision_Time	= 14-MAY-2024 19:50:28
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[dC]
X_90_Width	= 5.9[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 2.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]



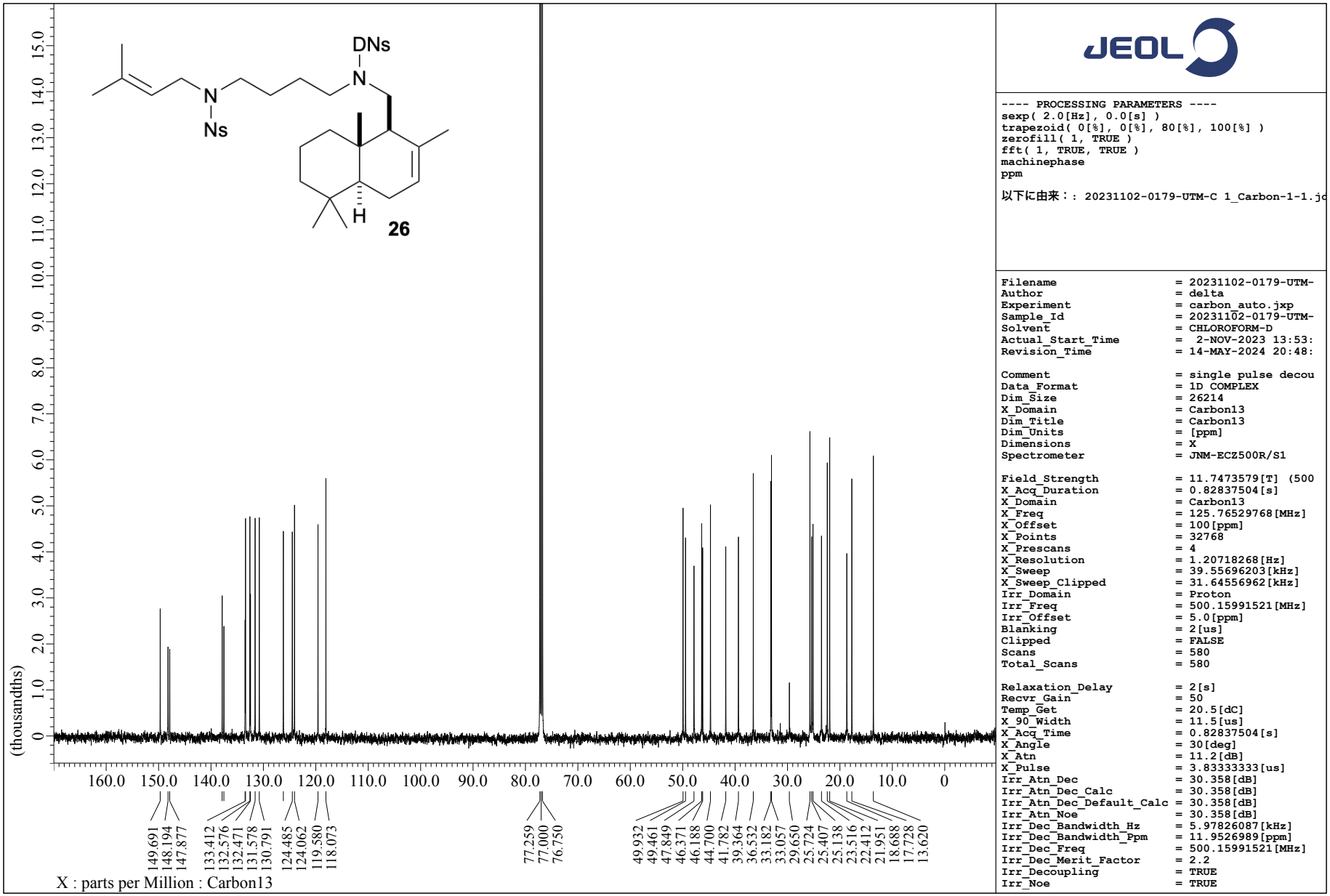

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 3.51605[%], 1 )

以下に由来：: 20230722-I-UTM-C_Carbon-1-1.jdf
```

Filename	= 20230722-I-UTM-C_C
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= 20230722-I-UTM-C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JUL-2023 01:04:
Revision_Time	= 14-MAY-2024 19:53:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 10000
Total_Scans	= 10000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.6[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.358[dB]
Irr_Atn_Dec_Calc	= 30.358[dB]
Irr_Atn_Dec_Default_Calc	= 30.358[dB]
Irr_Atn_Noe	= 30.358[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 2.43866[%], 1 )

以下に由来：: 20231102-0179-UTM 1_Proton-1-1.jdf
```

Filename	= 20231102-0179-UTM 1_P
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20231102-0179-UTM 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-NOV-2023 13:37:11
Revision_Time	= 14-MAY-2024 20:29:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.8[dC]
X_90_Width	= 6.25[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.125[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]


DNs
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26
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
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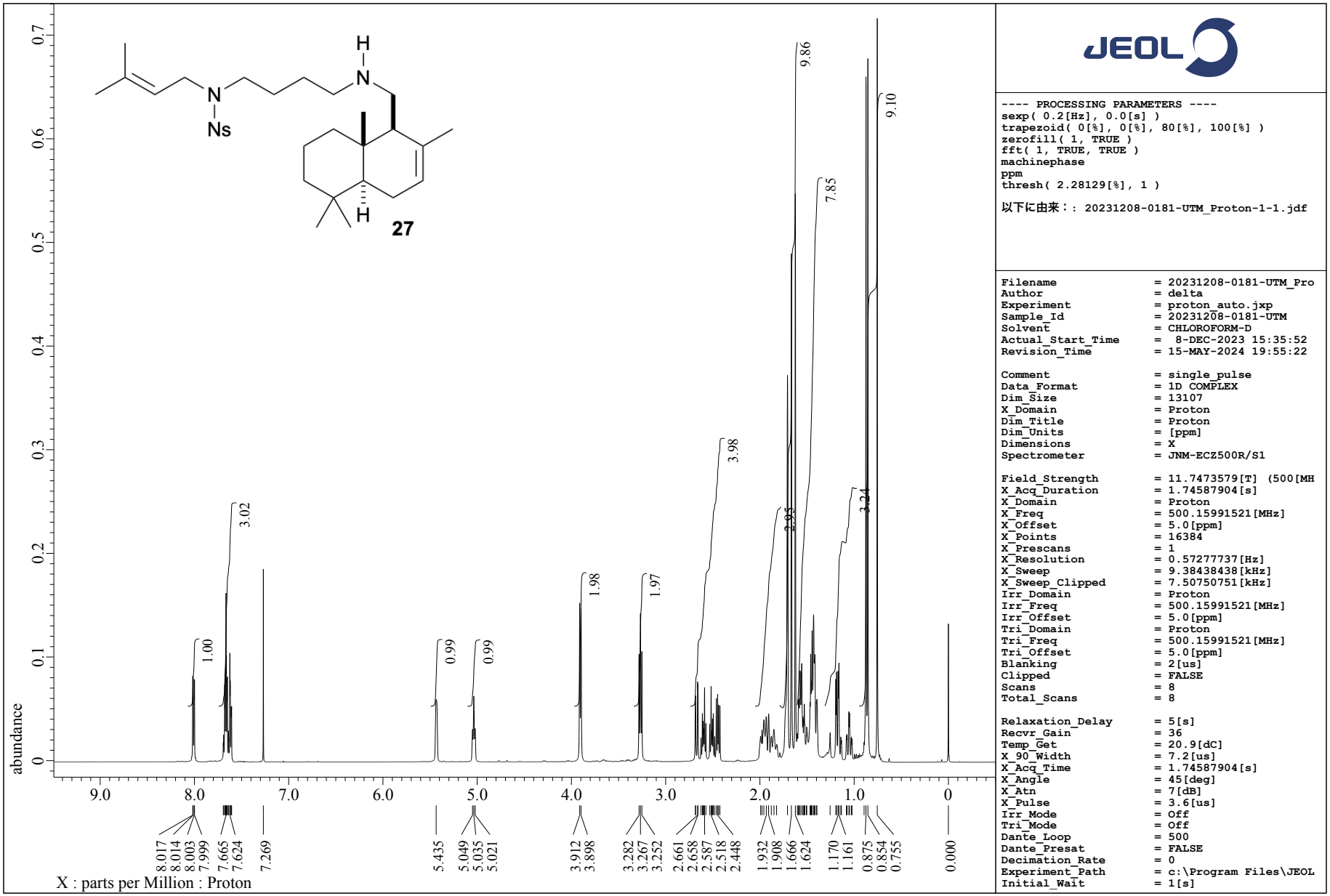
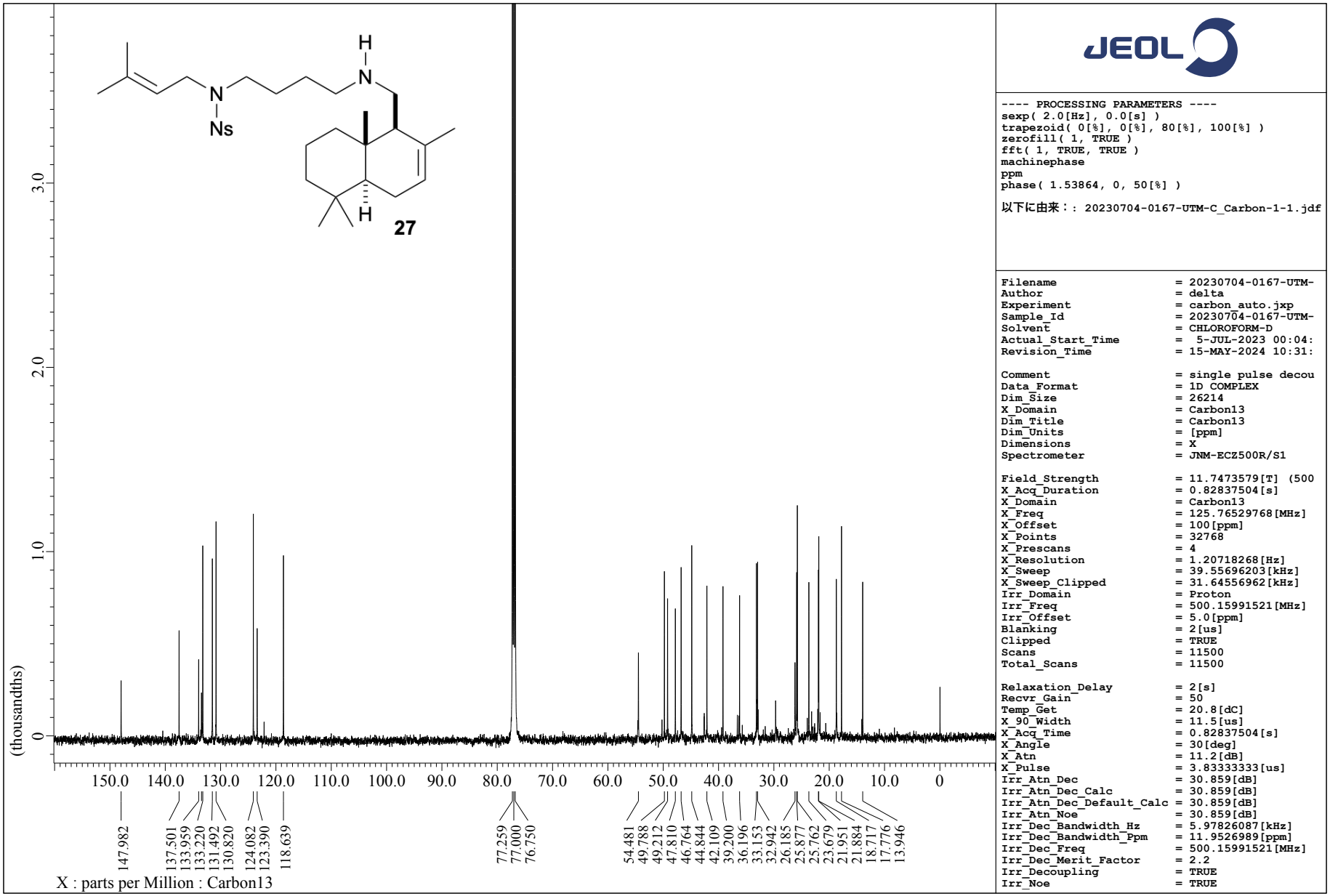
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
149.691
148.194
147.877
133.412
132.576
132.471
131.578
130.791
124.485
124.062
119.580
118.073
77.259
77.000
76.750
49.932
49.461
47.849
46.371
46.188
44.700
41.782
39.364
36.532
33.182
33.057
29.650
25.724
25.407
25.138
23.516
22.412
21.951
18.688
17.728
13.620
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来：: 20231102-0179-UTM-C 1_Carbon-1-1.jd
Filename = 20231102-0179-UTM-
Author = delta
Experiment = carbon_auto.jxp
Sample_Id = 20231102-0179-UTM-
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-NOV-2023 13:53:
Revision_Time = 14-MAY-2024 20:48:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.7473579[T] (500
X_Acq_Duration = 0.82837504[s]
X_Domain = Carbon13
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.20718268[Hz]
X_Sweep = 39.55696203[kHz]
X_Sweep_Clipped = 31.64556962[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 580
Total_Scans = 580
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.5[dC]
X_90_Width = 11.5[us]
X_Acq_Time = 0.82837504[s]
X_Angle = 30[deg]
X_Atn = 11.2[dB]
X_Pulse = 3.83333333[us]
Irr_Atn_Dec = 30.358[dB]
Irr_Atn_Dec_Calc = 30.358[dB]
Irr_Atn_Dec_Default_Calc = 30.358[dB]
Irr_Atn_Noe = 30.358[dB]
Irr_Dec_Bandwidth_Hz = 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.9526989[ppm]
Irr_Dec_Freq = 500.15991521[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE



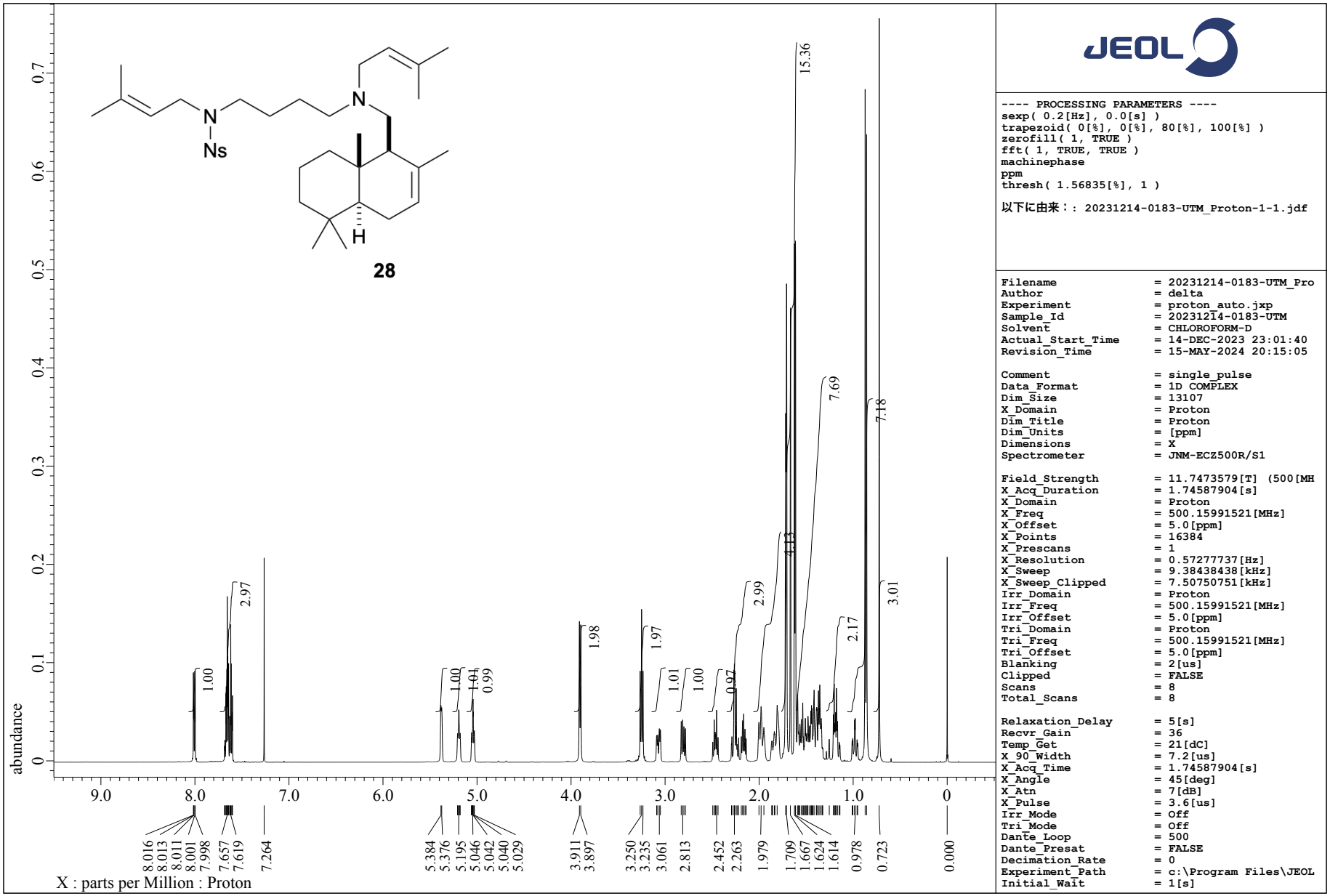

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 2.28129[%], 1 )

以下に由来：: 20231208-0181-UTM_Proton-1-1.jdf
```

Filename	= 20231208-0181-UTM_Pro
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20231208-0181-UTM
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-DEC-2023 15:35:52
Revision_Time	= 15-MAY-2024 19:55:22
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.9[dC]
X_90_Width	= 7.2[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.6[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]



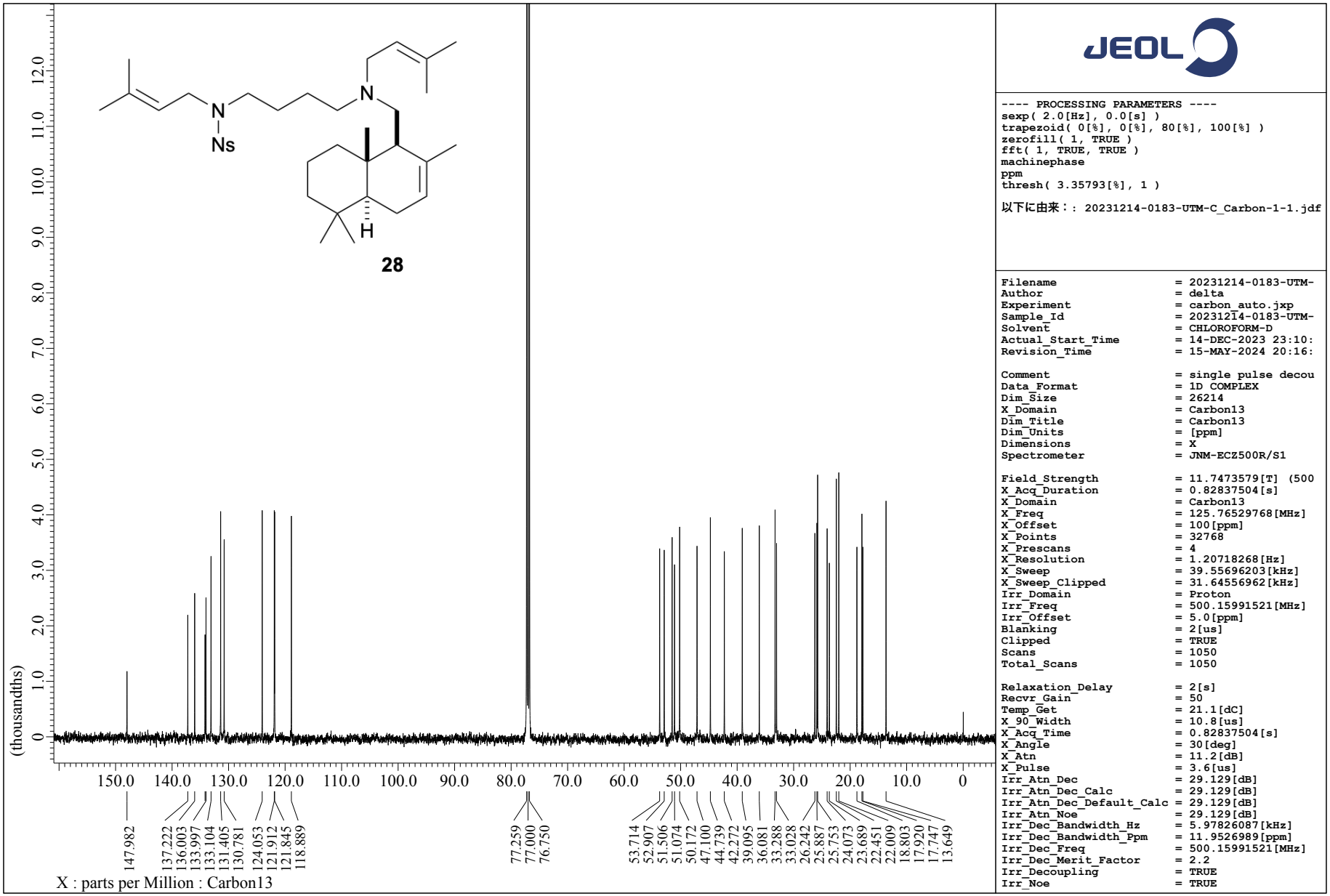

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 1.53864, 0, 50[%] )

以下に由来：: 20230704-0167-UTM-C_Carbon-1-1.jdf
```

Filename	= 20230704-0167-UTM-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= 20230704-0167-UTM-
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JUL-2023 00:04:
Revision_Time	= 15-MAY-2024 10:31:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 11500
Total_Scans	= 11500
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.8[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.859[dB]
Irr_Atn_Dec_Calc	= 30.859[dB]
Irr_Atn_Dec_Default_Calc	= 30.859[dB]
Irr_Atn_Noe	= 30.859[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



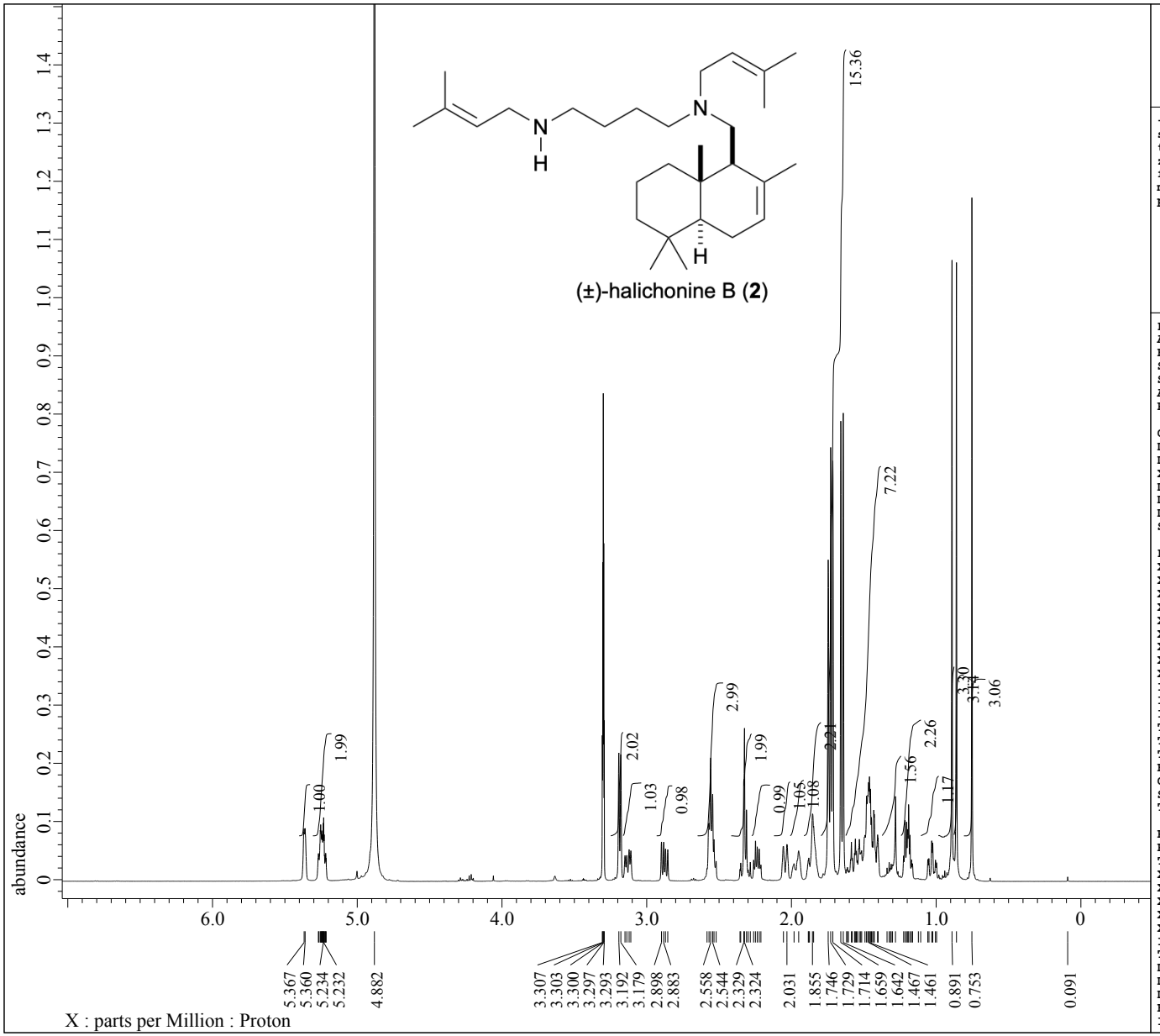

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 1.56835[%], 1 )

以下に由来：: 20231214-0183-UTM_Proton-1-1.jdf
```

Filename	= 20231214-0183-UTM_Pro
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20231214-0183-UTM
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-DEC-2023 23:01:40
Revision_Time	= 15-MAY-2024 20:15:05
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21[dC]
X_90_Width	= 7.2[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.6[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]



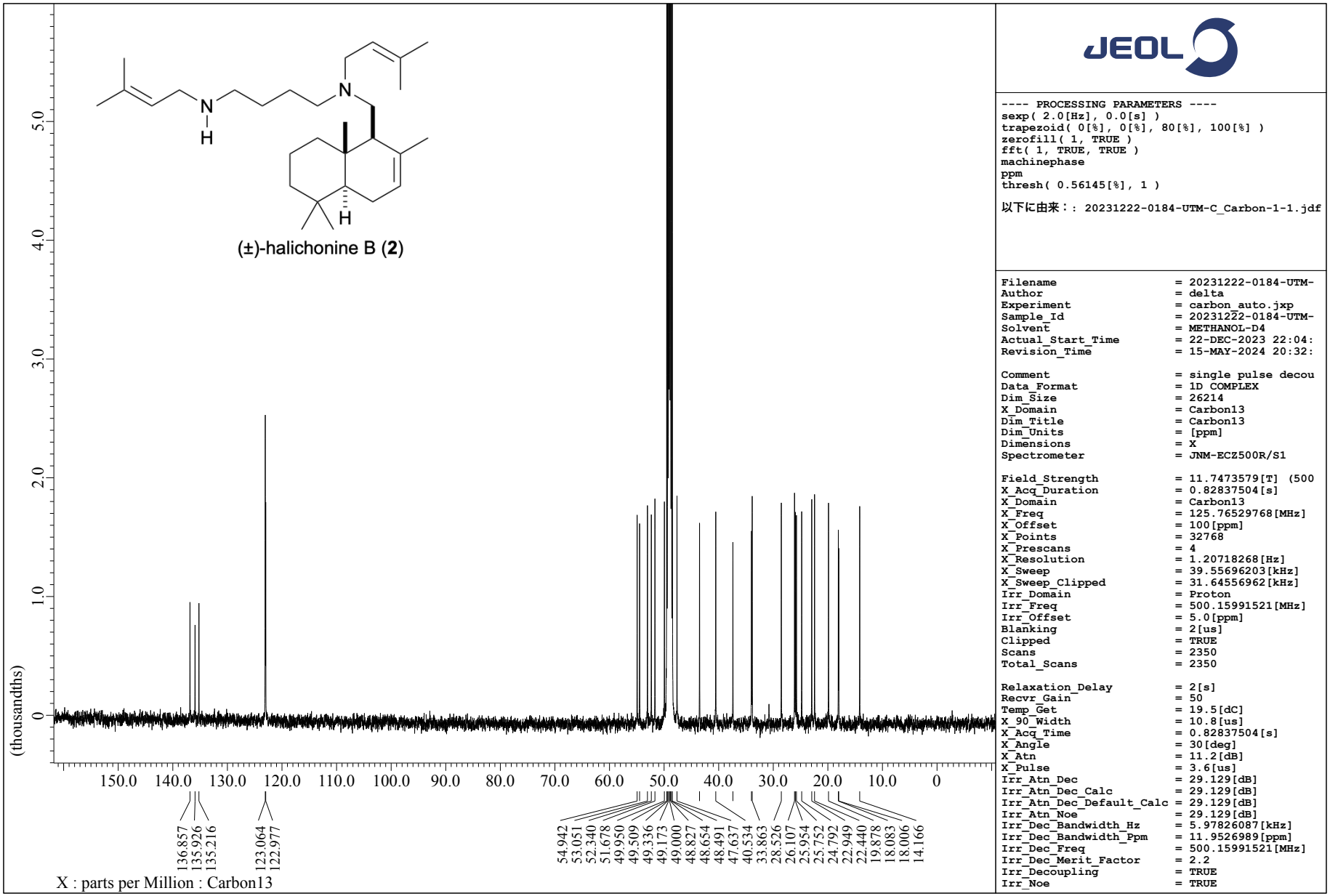

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 3.35793[%], 1 )

以下に由来：: 20231214-0183-UTM-C_Carbon-1-1.jdf
```

Filename	= 20231214-0183-UTM-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= 20231214-0183-UTM-
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-DEC-2023 23:10:
Revision_Time	= 15-MAY-2024 20:16:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 1050
Total_Scans	= 1050
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.1[dC]
X_90_Width	= 10.8[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.6[us]
Irr_Atn_Dec	= 29.129[dB]
Irr_Atn_Dec_Calc	= 29.129[dB]
Irr_Atn_Dec_Default_Calc	= 29.129[dB]
Irr_Atn_Noe	= 29.129[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE




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

Filename	= 20240106-0184-UTM-MeO
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= 20240106-0184-UTM-MeO
Solvent	= METHANOL-D4
Actual_Start_Time	= 7-JAN-2024 00:12:47
Revision_Time	= 15-MAY-2024 21:16:52
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500[MH
X_Acq_Duration	= 1.74587904[s]
X_Domain	= Proton
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
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	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 20.2[dC]
X_90_Width	= 7.2[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 7[dB]
X_Pulse	= 3.6[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 0.56145[%], 1 )

以下に由来：: 20231222-0184-UTM-C_Carbon-1-1.jdf
```

Filename	= 20231222-0184-UTM-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= 20231222-0184-UTM-
Solvent	= METHANOL-D4
Actual_Start_Time	= 22-DEC-2023 22:04:
Revision_Time	= 15-MAY-2024 20:32:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.7473579[T] (500
X_Acq_Duration	= 0.82837504[s]
X_Domain	= Carbon13
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.20718268[Hz]
X_Sweep	= 39.55696203[kHz]
X_Sweep_Clipped	= 31.64556962[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 2350
Total_Scans	= 2350
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.5[dC]
X_90_Width	= 10.8[us]
X_Acq_Time	= 0.82837504[s]
X_Angle	= 30[deg]
X_Atn	= 11.2[dB]
X_Pulse	= 3.6[us]
Irr_Atn_Dec	= 29.129[dB]
Irr_Atn_Dec_Calc	= 29.129[dB]
Irr_Atn_Dec_Default_Calc	= 29.129[dB]
Irr_Atn_Noe	= 29.129[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989[ppm]
Irr_Dec_Freq	= 500.15991521[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE