One-pot Synthesis of *trans*-2,3-Diaminoindolines through 2,3-Diamination of Electrophilic Indolines

Yuito Kobori[1], Keisuke Tokushige[1] and Takumi Abe*[1]

[1]Graduate School of Medicine, Dentistry and Pharmaceutical Sciences,
Okayama University, 1-1-1, Tsushima-naka, Kita-ku, Okayama 7008530, Japan
E-mail: t-abe@okayama-u.ac.jp

Supporting Information

General methods. Column chromatography was carried out using silica gel (WAKO Gel 75–150 mesh, WAKO Co., Ltd.). Preparative tin-layer chromatography was performed with silica gel plates (60F-254). Melting points (mp) were recorded with a Yamato melting point apparatus model MP-21 and are uncorrected. IR spectra were measured with a HORIBA fourier transform infrared spectrometer FT-720, and absorbance frequencies are reported in reciprocal centimeters (cm^{-1}). NMR experiments were performed with JEOL JNM-ECZ600R (^1H NMR: 600 MHz, ^{13}C NMR: 151 MHz) spectrometer and Varian NMR system 600 (^1H NMR:600 MHz, ^{13}C NMR: 151 MHz) spectrometer. Chemical shifts are expressed in δ (parts per million, ppm) calues, and coupling constants are expressed in herts (Hz). ^1H NMR spectra were referenced to a solvent signal ($CDCl_3$: 7.26 ppm, DMSO-d_6: 2.50 ppm). ^{13}C NMR spectra were referenced to a solvent signal ($CDCl_3$: 77.1 ppm, DMSO-d_6: 39.5). Signal multiplicities are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), doublet of doublets (dd), doublet of doublet of doublets (ddd) septet (sept), broad (br). High-resolution MS spectra were recorded with a Brucker microTOF mass spectrometers (ESI-TOF-MS). Reactions were monitored by thin layer chromatography (TLC) carried out on a silica gel plates (60F-254) and visualized under UV illumination at 254 or 365 nm depending on the compounds.

Compound number of amines to be used in this reaction

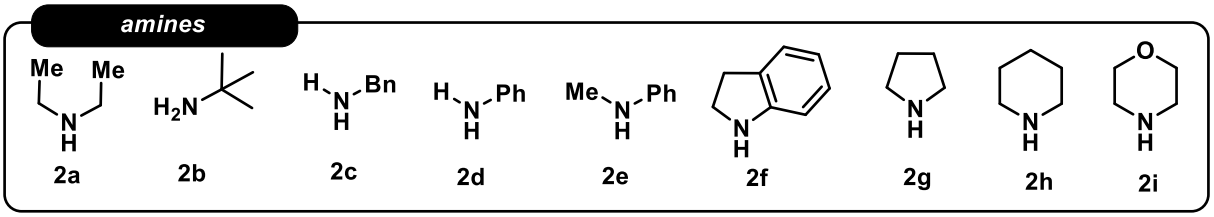


Figure S1.

Synthesis of *N*-protected indoles S1

The *N*-protected indoles **S1** as *N*-tosylindoles (**S1a**, **S1e–S1j**), *N*-benzenesulfonylindole (**S1b**), *N*-(4-methoxybenzenesulfonyl)indole (**S1c**) and *N*-(4-phenylbenzenesulfonyl)indole (**S1d**) were prepared by reported method.[2] All substrates were used as received from commercial suppliers (Sigma-Aldrich, Kanto Chemical, TCI, Wako and Nacalai tesque) and all reagents were weighed and handled in air at room temperature. Analytical data are in accordance with the literature values.[2]

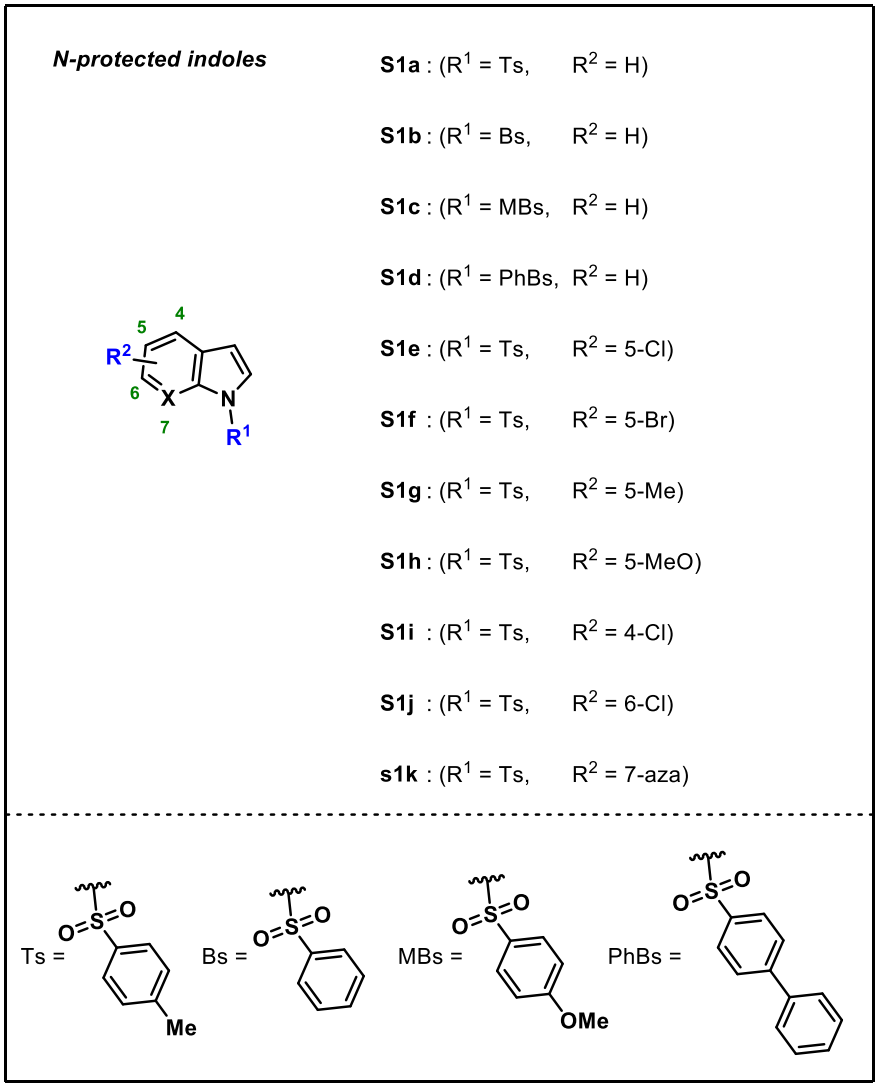


Figure S2.

Synthesis of *trans*-2-hydroxyindoline-3-trirthylammonium bromide (HITAB) 1

The *trans*-2-hydroxyindoline-3-triethylammonium bromides (HITAB) **1** were prepared by reported method.[3] All reagents were weighed and handled in air at room temperature. Analytical data are in accordance with the literature values (1a[3a], 1b, 1f, 1j[3b], 1c[3c], 1e, and 1h[3d]).

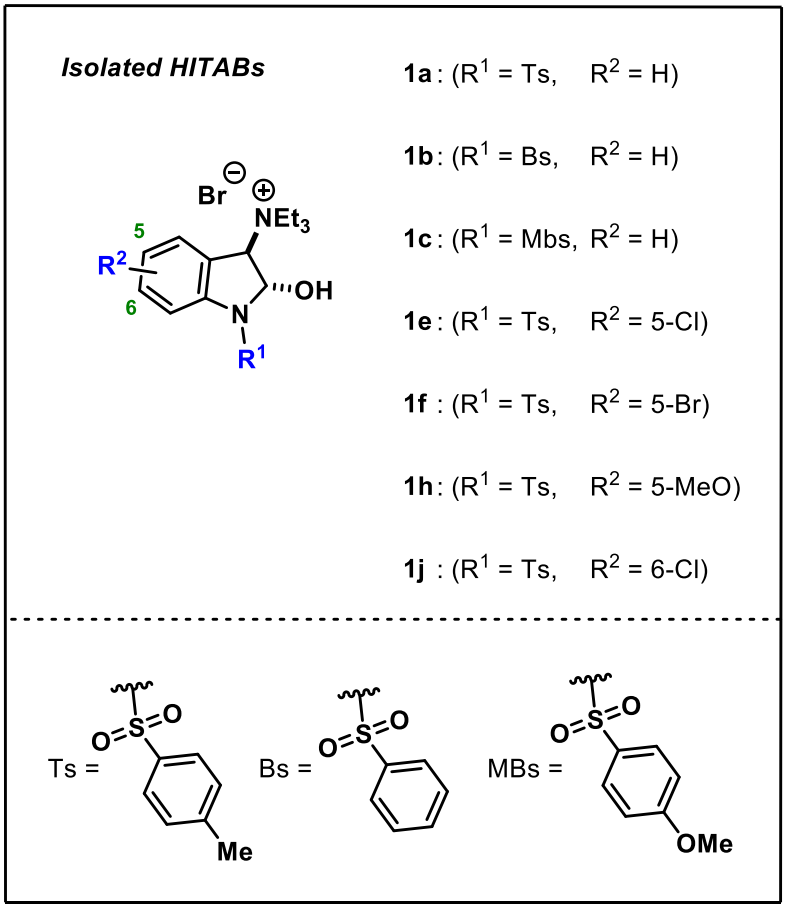
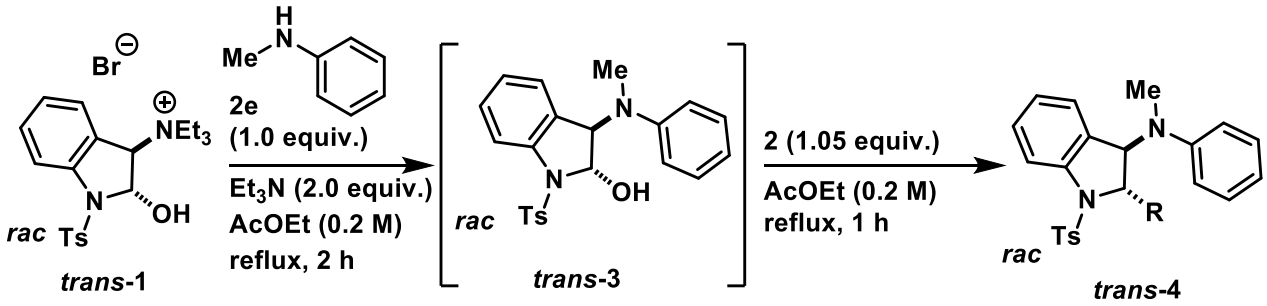


Figure S3.

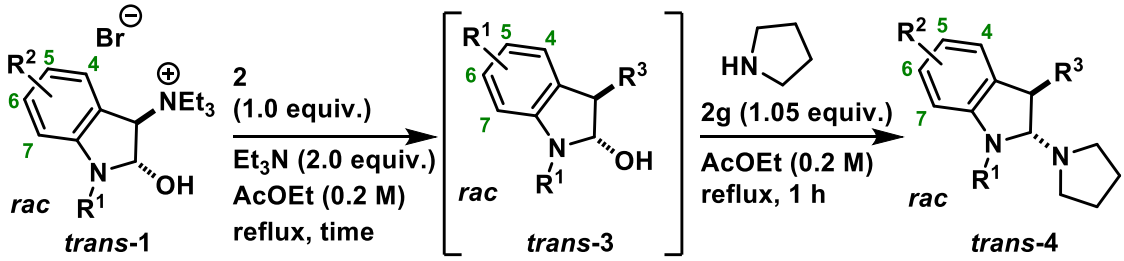
Synthesis of *trans*-2,3-diaminoindolines 4

Scheme S2: Typical procedure for Table 1



This reaction was performed with the synthesis of **4aec** (R = **2c**), **4aeg** (R = **2g**), **4aeh** (R = **2h**), and **4aei** (R = **2i**). To a mixture of **1** (469 mg, 1.0 equiv., 1.0 mmol) and **2e** (0.108 mL, 1.0 equiv., 1.0 mmol) in AcOEt (5.0 mL, 0.2 M) was added Et_3N (0.277 mL, 2.0 equiv. 2.0 mmol). The mixture was stirred at reflux for 2 h. After the whole was cooled to room temperature, **2** (1.05 equiv., 1.05 mmol) was added to the mixture and stirred at reflux further 1 h. After the whole was cooled to room temperature, H_2O (20 mL) was added to the mixture. The whole was extracted with AcOEt (3 x 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by recrystallization or silica gel column chromatography.

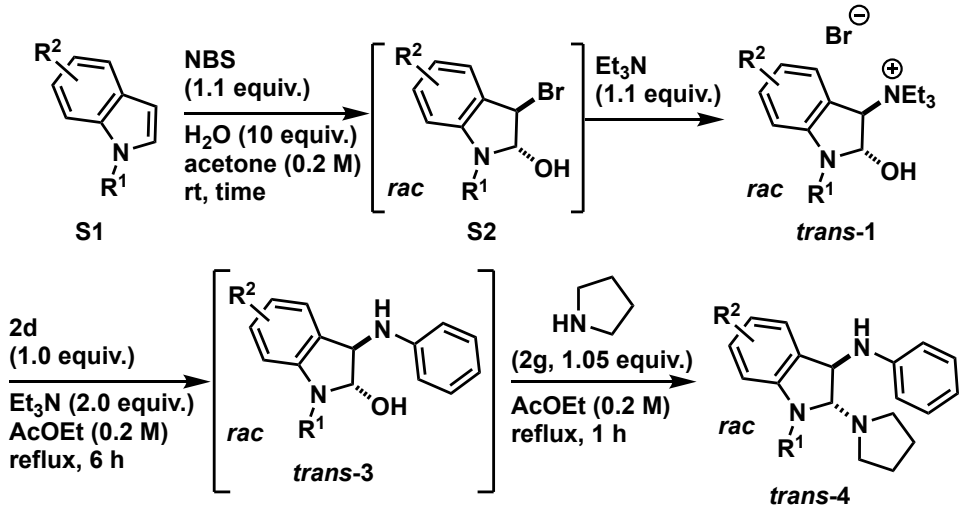
Scheme S3: General procedure A



This reaction was performed with the synthesis of **4adg** (R^1 = Ts, R^2 = H, R^3 = **2d**), **4bdg** (R^1 = Bs, R^2 = H, R^3 = **2d**), **4cdg** (R^1 = MBs, R^2 = H, R^3 = **2d**), **4edg** (R^1 = Ts, R^2 = 5-Cl, R^3 = **2d**), **4fdg** (R^1 = Ts, R^2 = 5-Br, R^3 = **2d**), **4hdg** (R^1 = Ts, R^2 = 5-MeO, R^3 = **2d**), **4jdg** (R^1 = Ts, R^2 = 6-Cl, R^3 = **2d**), **4ajg** (R^1 = Ts, R^2 = H, R^3 = **2j**), **4akg** (R^1 = Ts, R^2 = H, R^3 = **2k**), **4alg** (R^1 = Ts, R^2 = H, R^3 = **2l**), **4amg** (R^1 = Ts, R^2 = H, R^3 = **2m**), **4ang** (R^1 = Ts, R^2 = H, R^3 = **2n**), **4aog** (R^1 = Ts, R^2 = H, R^3 = **2o**), **4apg** (R^1 = Ts, R^2 = H, R^3 = **2p**), **4aqg** (R^1 = Ts, R^2 = H, R^3 = **2q**), **4afg** (R^1 = Ts, R^2 = H, R^3 = **2f**), **4agg** (R^1 = Ts, R^2 = H, R^3 = **2g**), **4ahg** (R^1 = Ts, R^2 = H, R^3 = **2h**), **4aig** (R^1 = Ts, R^2 = H, R^3 = **2i**), **4abg** (R^1 = Ts, R^2 = H, R^3 = **2b**), and **4arg** (R^1 = Ts, R^2 = H, R^3 = **2r**).

To a mixture of **1** (469 mg, 1.0 equiv., 1.0 mmol) and **2** (1.0 equiv., 1.0 mmol) in AcOEt (5.0 mL, 0.2 M) was added Et_3N (0.277 mL, 2.0 equiv. 2.0 mmol). The mixture was stirred at reflux for 1–6 h. After the whole was cooled to room temperature, **2g** (0.088 mL, 1.05 equiv., 1.05 mmol) was added to the mixture and stirred at reflux further 1 h. After the whole was cooled to room temperature, H_2O (20 mL) was added to the mixture. The whole was extracted with AcOEt (3 x 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by recrystallization or silica gel column chromatography.

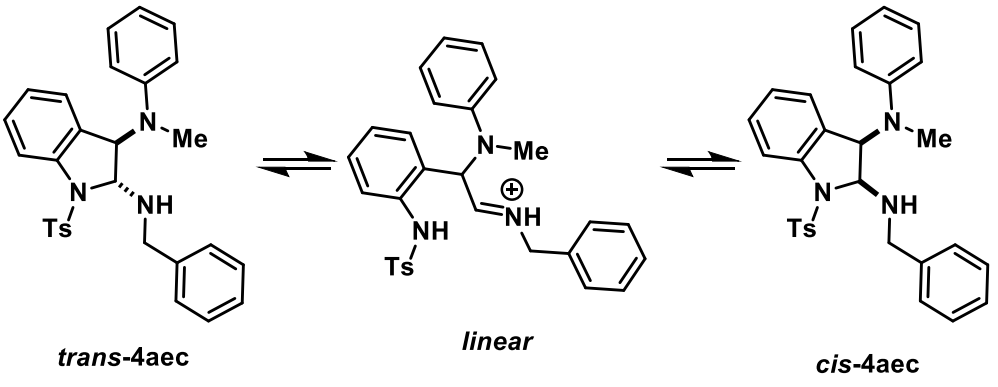
Scheme S4: General procedure B



This reaction was performed with the synthesis of **4ddg** (R^1 = PhBs, R^2 = H), **4gdg** (R^1 = Ts, R^2 = 5-Me), and **4idg** (R^1 = Ts, R^2 = 4-Cl).

To a solution of **S1** (1.0 equiv., 1.0 mmol) and H_2O (0.18 mL, 10 equiv., 10 mmol) in acetone (5.0 mL, 0.2 M) was added NBS (196 mg, 1.1 equiv., 1.1 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material indicated by TLC. Then Et_3N (0.152 mL, 1.1 equiv. 1.1 mmol) was added to the mixture and stirred further 0.5 h. After the mixture was concentrated *in vacuo*, the residue was dissolved in AcOEt (5.0 mL, 0.2 M). To this mixture was added aniline **2d** (0.091 mL, 1.0 equiv., 1.0 mmol) and Et_3N (0.277 mL, 2.0 equiv., 2.0 mmol). The mixture was stirred at reflux for 6 h. After the whole was cooled to room temperature, pyrrolidine **2d** (0.086 mL, 1.05 equiv., 1.05 mmol) was added to the mixture and stirred at reflux further 1 h. After the whole was cooled to room temperature, H_2O (20 mL) was added to the mixture. The whole was extracted with AcOEt (3 x 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by recrystallization or silica gel column chromatography.

***trans*-N^2-Benzyl-N^3-methyl-N^3-phenyl-1-tosylindoline-2,3-diamine (4aec)**



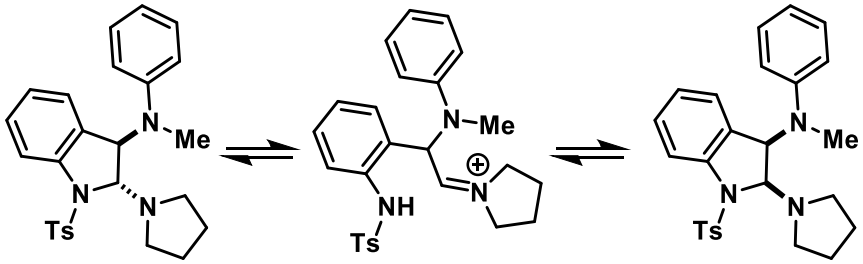
(*trans*:*cis* = >20:<1)

The reaction was performed according to the typical procedure for Table S1 using 0.108 mL (1.05 mmol) of **2c**. The residue was purified by silica-gel column chromatography using hexane/AcOEt (20/1–10/1 [v/v]) and

recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4aec** (306 mg, 0.63 mmol, 63% yield) as a white solid.

White solid (306 mg, 0.63 mmol, 63% yield; mp 116–118 °C); IR (KBr) ν: 3367, 3057, 3032, 2943, 2866, 2812, 1350, 1167, 754, 698 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 8.4 Hz, 1H), 7.71 (d, J = 8.4 Hz, 2H), 7.40–7.42 (m, 3H), 7.35 (t, J = 7.5 Hz, 2H), 7.26–7.30 (m, 3H), 7.22 (d, J = 8.4 Hz, 2H), 7.06–7.11 (m, 2H), 6.95 (d, J = 8.4 Hz, 2H), 6.83 (t, J = 7.2 Hz, 1H), 5.16 (d, J = 3.0 Hz, 1H), 5.06 (d, J = 3.6 Hz, 1H), 4.06 (d, J = 13.8 Hz, 1H), 3.81 (d, J = 13.2 Hz, 1H), 2.39 (s, 3H), 1.77 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 149.6, 144.4, 141.9, 139.9, 135.4, 130.1, 129.9, 129.3, 128.8, 128.5, 128.4, 127.3, 127.2, 126.3, 124.3, 118.0, 115.7, 114.1, 82.5, 65.0, 46.7, 32.3, 21.6; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{29}H_{29}N_3O_2SNa$ 506.1878; Found 506.1875.

***trans*-*N*-Methyl-*N*-phenyl-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4aeg)**

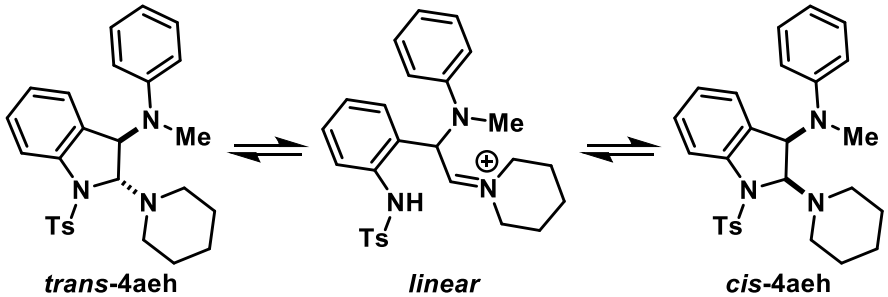


(*trans*:*cis* = >20:<1)

The reaction was performed according to the typical procedure for Table S1 using 0.086 mL (1.05 mmol) of **2g**. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4aeg** (409 mg, 0.91 mmol, 91% yield) as a white solid.

White solid (409 mg, 0.91 mmol, 91% yield; mp 128–130 °C, dec.); IR (KBr) ν: 3057, 3024, 2968, 2916, 2868, 2827, 1350, 1167, 752, 696 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, J = 7.8 Hz, 1H), 7.63 (d, J = 8.4 Hz, 2H), 7.37 (ddd, J = 8.4, 6.6, 1.8 Hz, 1H), 7.29 (t, J = 8.7 Hz, 2H), 7.14 (d, J = 8.4 Hz, 2H), 7.06–7.10 (m, 2H), 6.93 (d, J = 7.8 Hz, 2H), 6.81 (t, J = 7.2 Hz, 1H), 5.21 (d, J = 1.2 Hz, 1H), 4.87 (s, 1H), 2.84–2.88 (m, 2H), 2.59–2.63 (m, 2H), 2.34 (s, 3H), 1.71–1.80 (m, 4H), 1.64 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 149.5, 143.9, 142.7, 136.4, 130.1, 129.65, 129.65, 129.4, 127.6, 126.7, 124.5, 117.6, 116.7, 113.4, 86.3, 65.4, 47.2, 32.3, 23.8, 21.6; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{26}H_{29}N_3O_2SNa$ 470.19878; Found 470.1883.

***trans*-*N*-Methyl-*N*-phenyl-2-(piperidin-1-yl)-1-tosylindolin-3-amine (4aeh)**

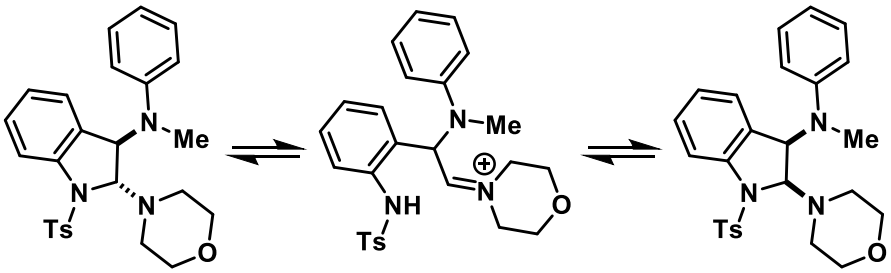


(*trans*:*cis* = >20:<1)

The reaction was performed according to the typical procedure for Table S1 using 0.104 mL (1.05 mmol) of **2h**. The residue was purified by silica-gel column chromatography using hexane/chloroform (1/2 [v/v]) and recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4aeh** (85 mg, 0.18 mmol, 18% yield) as a white solid.

White solid (85 mg, 0.18 mmol, 18% yield; mp 154–156 °C, dec.); IR (KBr) ν: 3068, 3051, 3012, 2937, 2912, 2848, 2816, 1354, 1169, 750, 696 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, J = 7.8 Hz, 1H), 7.62 (d, J = 8.4 Hz, 2H), 7.36 (td, J = 8.4, 1.8 Hz, 1H), 7.29 (t, J = 9.0 Hz, 2H), 7.15 (d, J = 7.8 Hz, 2H), 7.07 (td, J = 7.5, 0.6 Hz, 1H), 7.05 (d, J = 8.4 Hz, 1H), 7.01 (d, J = 7.8 Hz, 2H), 6.81 (t, J = 7.2 Hz, 1H), 4.89 (s, 1H), 4.83 (d, J = 2.4 Hz, 1H), 2.57–2.67 (m, 4H), 2.34 (s, 3H), 1.68 (s, 3H), 1.52–1.63 (m, 4H), 1.45-1.49 (m, 2H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 149.7, 144.0, 142.9, 136.3, 130.1, 130.0, 129.7, 129.3, 127.6, 126.1, 124.4, 117.6, 116.8, 113.8, 90.2, 65.8, 49.3, 32.4, 26.6, 24.5, 21.6; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{27}H_{31}N_3O_2SNa$ 484.2035; Found 484.2039.

***trans*-*N*-Methyl-2-morpholino-*N*-phenyl-1-tosylindolin-3-amine (4aei)**

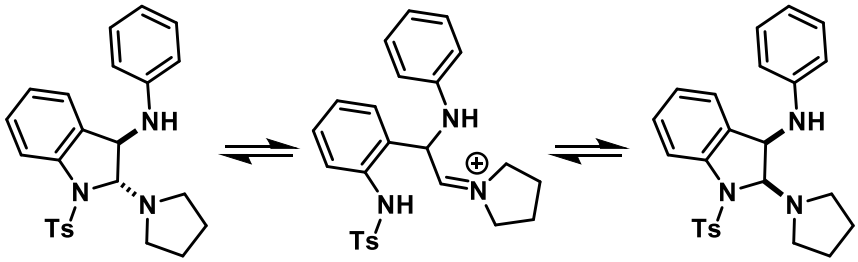


(*trans*:*cis* = >20:<1)

The reaction was performed according to the typical procedure for Table S1 using 0.091 mL (1.05 mmol) of **2i**. The residue was purified by silica-gel column chromatography using hexane/acetone (5/1–3/1 [v/v]) and recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4aei** (18 mg, 0.04 mmol, 4% yield) as a white solid.

White solid (18 mg, 0.04 mmol, 4% yield; mp 146–148 °C, dec.); IR (KBr) ν: 2958, 2924, 2852, 1346, 1167, 748, 694 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, J = 7.8 Hz, 1H), 7.64 (d, J = 9.0 Hz, 2H), 7.38 (td, J = 8.4, 1.5 Hz, 1H), 7.30 (t, J = 8.7 Hz, 2H), 7.16 (d, J = 7.8 Hz, 2H), 7.10 (td, J = 7.5, 0.6 Hz, 1H), 7.07 (d, J = 7.2 Hz, 1H), 6.99 (d, J = 8.4 Hz, 2H), 6.83 (t, J = 7.2 Hz, 1H), 4.92 (s, 1H), 4.84 (d, J = 1.8 Hz, 1H), 3.66–3.75 (m, 4H), 2.61–2.70 (m, 4H), 2.35 (s, 3H), 1.70 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 149.3, 144.1, 142.6, 136.1, 130.1, 129.61, 129.61, 129.3, 127.5, 126.1, 124.5, 117.7, 116.7, 113.6, 88.7, 67.2, 65.1, 48.3, 32.2, 21.5; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{26}H_{29}N_3O_3SNa$ 486.1827; Found 486.1829.

***trans*-*N*-Phenyl-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4adg)**

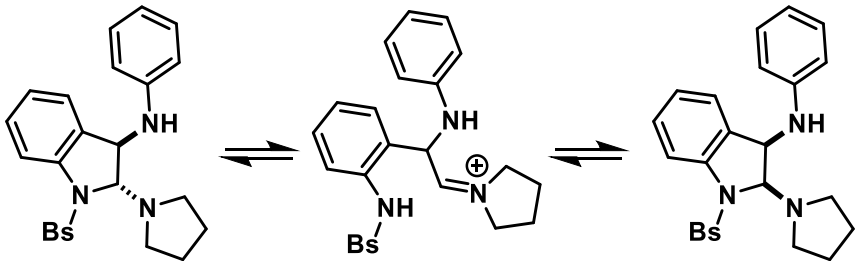


trans*-4adg** ***linear ***cis*-4adg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 0.091 mL (1.0 mmol) of **2d** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4adg** (383 mg, 0.88 mmol, 88% yield) as a white solid.

White solid (383 mg, 0.88 mmol, 88% yield; mp 126–128 °C, dec.); IR (KBr) ν: 3419, 3086, 3014, 2970, 2910, 2881, 2844, 1348, 1157, 756, 706 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, J = 8.4 Hz, 1H), 7.41 (d, J = 9.0 Hz, 2H), 7.38 (td, J = 8,7, 1.5 Hz, 1H), 7.19–7.21 (m, 3H), 7.11 (td, J = 7.5, 0.6 Hz, 1H), 7.09 (d, J = 8.4 Hz, 2H), 6.77 (t, J = 7.5 Hz, 1H), 6.42 (d, J = 7.8 Hz, 2H), 5.15 (s, 1H), 4.50 (d, J = 7.2 Hz, 1H), 2.76–2.80 (m, 2H), 2.54–2.57 (m, 2H), 2.41 (d, J = 7.2 Hz, 1H), 2.38 (s, 3H), 1.71–1.78 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 145.6, 143.8, 142.7, 135.1, 132.5, 130.3, 129.5, 129.4, 127.4, 125.6, 125.4, 118.2, 117.7, 113.3, 85.7, 59.8, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{27}N_3O_2SNa$ 456.1722; Found 456.1722.

***trans*-*N*-Phenyl-1-(phenylsulfonyl)-2-(pyrrolidin-1-yl)indolin-3-amine (4bdg)**

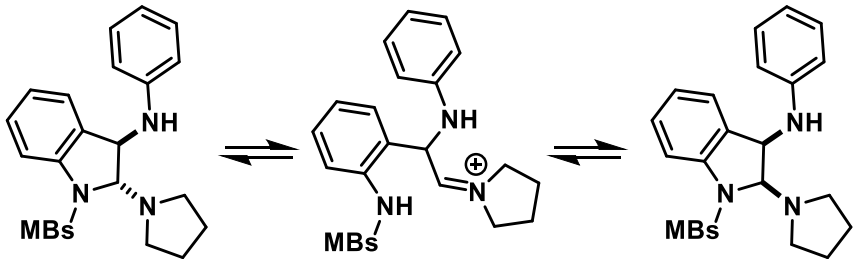


trans*-4bdg** ***linear ***cis*-4bdg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 455 mg (1.0 mmol) of **1b** and 0.091 mL (1.0 mmol) of **2d** for 3 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4bdg** (345 mg, 0.82 mmol, 82% yield) as a white solid.

White solid (345 mg, 0.82 mmol, 82% yield; mp 130–132 °C, dec.); IR (KBr) ν: 3423, 3072, 3041, 2974, 2929, 2877, 2848, 1350, 1169, 750, 721 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 7.8 Hz, 1H), 7.54 (d, J = 7.8 Hz, 2H) 7.52 (t, J = 7.2 Hz, 1H), 7.39 (td, J = 8.4, 1.2 Hz, 1H), 7.31 (t, J = 8.1 Hz, 2H), 7.21 (d, J = 7.2 Hz, 1H), 7.20 (d, J = 7.8 Hz, 2H), 7.12 (td, J = 7.8, 1.2 Hz, 1H), 6.77 (t, J = 7.2 Hz, 1H), 6.44 (d, J = 7.8 Hz, 2H), 5.18 (s, 1H), 4.50 (d, J = 7.2 Hz, 1H), 2.77–2.80, (m, 2H), 2.55–2.58 (m, 2H), 2.40 (d, J = 7.2 Hz, 1H), 1.72–1.76 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 145.5, 142.5, 138.0, 133.0, 132.5, 130.3. 129.5, 128.9, 127.4, 125.6, 125.5, 118.2, 117.7, 113.3, 85.9, 59.8, 47.5, 23.5; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{24}H_{25}N_3O_2SNa$ 442.1565; Found 442.1566.

***trans*-1-((4-Methoxyphenyl)sulfonyl)-*N*-phenyl-2-(pyrrolidin-1-yl)indolin-3-amine (4cdg)**

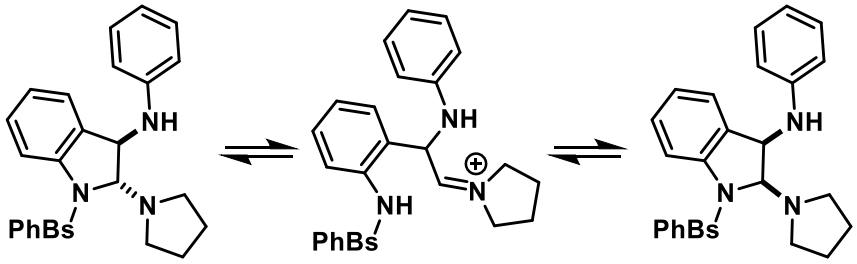


trans*-4cdg** ***linear ***cis*-4cdg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 485 mg (1.0 mmol) of **1c** and 0.091 mL (1.0 mmol) of **2d** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4cdg** (333 mg, 0.74 mmol, 74% yield) as a white solid.

White solid (333 mg, 0.74 mmol, 74% yield; mp 126–128 °C, dec.); IR (KBr) ν: 3413, 3072, 3026, 2970, 2931, 2871, 2841, 1346, 1259, 1157, 1024, 754, 698 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, J = 7.8 Hz, 1H), 7.45 (d, J = 9.6 Hz, 2H), 7.38 (td, J = 8.4, 1.2 Hz, 1H), 7.21 (d, J = 7.2 Hz, 2H), 7.20 (d, J = 8.4 Hz, 1H), 7.11 (td, J = 7.2, 0.9 Hz, 1H), 6.77 (t, J = 7.2 Hz, 1H), 6.75 (d, J = 9.0 Hz, 2H), 6.46 (d, J = 7.2 Hz, 2H), 5.14 (s, 1H), 4.49 (d, J = 7.2 Hz, 1H), 3.82 (s, 3H), 2.77–2.79 (m, 2H), 2.54–2.57 (m, 2H), 2.50 (d, J = 6.6 Hz, 1H), 1.71–1.78 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 163.0, 145.7, 142.8, 132.5, 130.3, 129.8, 129.47, 129.47, 125.5, 125.3, 118.1, 117.8, 113.9, 113.2, 85.6, 59.8, 55.7, 47.5, 23.4; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{27}N_3O_3SNa$ 472.1671; Found 472.1671.

***trans*-1-([1,1'-Biphenyl]-4-ylsulfonyl)-*N*-phenyl-2-(pyrrolidin-1-yl)indolin-3-amine (4ddg)**



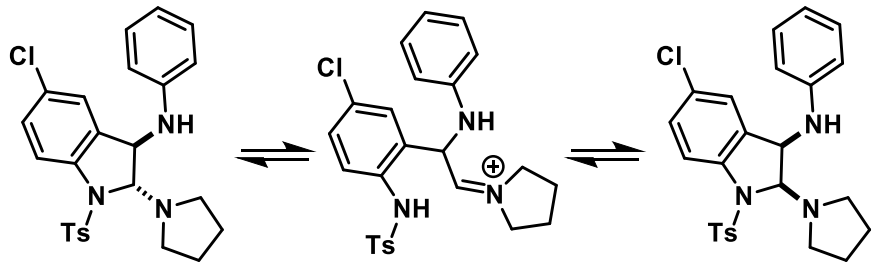
trans*-4ddg** ***linear ***cis*-4ddg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure B using 333 mg (1.0 mmol) of **1d** and 0.091 mL (1.0 mmol) of **2d**. The residue was purified by silica-gel column chromatography using hexane/AcOEt (10/1 [v/v]) and recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4ddg** (136 mg, 0.27 mmol, 27% yield) as a pale purple solid.

Pale purple solid (136 mg, 0.27 mmol, 27% yield; mp 134–136 °C, dec.); IR (KBr) ν: 3392, 3057, 3026, 2964, 2924, 2877, 2848, 1352, 1167, 756, 694 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, J = 7.8 Hz, 1H), 7.57–7.59 (m, 4H), 7.52 (d, J = 8.4 Hz, 2H), 7.48 (t, J = 7.5 Hz, 2H), 7.43 (d, J = 7.2 Hz, 1H), 7.41 (td, J = 7.2, 0.9 Hz, 1H), 7.22 (d, J = 6.6 Hz, 1H), 7.18 (t, J = 7.2 Hz, 2H), 7.14 (td, J = 7.2, 0.9 Hz, 1H), 6.76 (t, J = 7.2 Hz, 1H), 6.40 (d, J = 7.2 Hz, 2H), 5.20 (s, 1H), 4.51 (d, J = 6.6 Hz, 1H), 2.79–2.82 (m, 2H), 2.57–2.59 (m, 2H), 2.48 (d, J = 6.6 Hz, 1H), 1.75–1.77 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 145.53, 145.47, 142.5, 138.9,

136.5, 132.5, 130.3, 129.4, 129.2, 128.7, 127.8, 127.20, 127.20, 125.53, 125.47, 118.1, 117.7, 113.2, 85.7, 59.8, 47.5, 23.5; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{30}H_{29}N_3O_2SNa$ 518.1878; Found 518.1883.

***trans*-5-Chloro-*N*-phenyl-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4edg)**

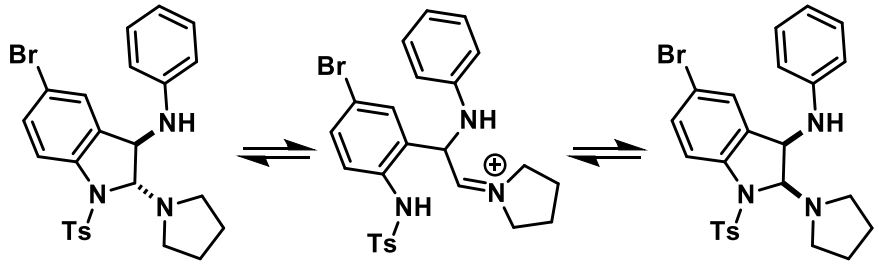


trans*-4edg** ***linear ***cis*-4edg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 504 mg (1.0 mmol) of **1e** and 0.091 mL (1.0 mmol) of **2d** for 3 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4edg** (426 mg, 0.91 mmol, 91% yield) as a white solid.

White solid (426 mg, 0.91 mmol, 91% yield; mp 131–133 °C, dec.); IR (KBr) ν: 3408, 3055, 3028, 2972, 2922, 2860, 2823, 1352, 1169, 1090, 754, 696 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, J = 9.0 Hz, 1H), 7.41 (d, J = 8.4 Hz, 2H), 7.34 (dd, J = 8.7, 2.1 Hz, 1H), 7.21 (t, J = 7.5 Hz, 2H), 7.18 (d, J = 2.4 Hz, 1H), 7.12 (d, J = 7.8 Hz, 2H), 6.79 (t, J = 7.5 Hz, 1H), 6.41 (d, J = 7.8 Hz, 2H), 5.15 (s, 1H), 4.47 (d, J = 7.8 Hz, 1H), 2.76–2.79 (m, 2H), 2.53–2.56 (m, 2H), 2.41 (s, 3H), 1.73–1.78 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 145.3, 144.1, 141.3, 134.9, 134.1, 130.44, 130.40, 129.7, 129.5, 127.4, 125.8, 118.8, 118.5, 113.3, 86.1, 59.6, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}ClN_3O_2SNa$ 490.1332, 492.1302; Found 490.1328, 492.1297.

***trans*-5-Bromo-*N*-phenyl-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4fdg)**



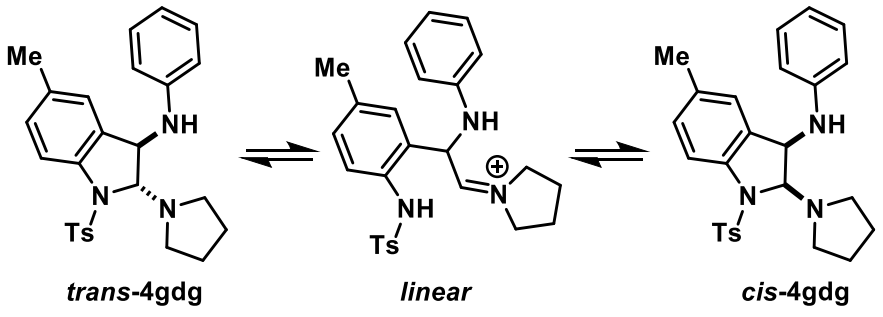
trans*-4fdg** ***linear ***cis*-4fdg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 548 mg (1.0 mmol) of **1f** and 0.091 mL (1.0 mmol) of **2d** for 3 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4fdg** (469 mg, 0.92 mmol, 92% yield) as a pale beige solid.

Pale beige solid (469 mg, 0.92 mmol, 92% yield; mp 130–132 °C, dec.); IR (KBr) ν: 3408, 3055, 3028, 2970, 2922, 2860, 2821, 1352, 1167, 754, 696 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, J = 8.4 Hz, 1H), 7.49 (dd, J = 6.0, 2.4 Hz, 1H), 7.41 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 1.8 Hz, 1H), 7.21 (t, J = 7.8 Hz, 2H), 7.12 (d, J = 7.8 Hz, 2H), 6.79 (t, J = 7.5 Hz, 1H), 6.41 (d, J = 7.2 Hz, 2H), 5.15 (s, 1H), 4.47 (d, J = 7.2 Hz, 1H), 2.76–2.79 (m, 2H), 2.53–2.56 (m, 2H), 2.41 (s, 3H), 1.74–1.77 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 145.3, 144.1,

141.8, 134.9, 134.5, 133.3, 129.7, 129.5, 128.7, 127.4, 119.2, 118.5, 117.9, 113.3, 86.1, 59.5, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}BrN_3O_2SNa$ 534.0827, 536.0806; Found 534.0827, 536.0810.

***trans*-5-Methyl-*N*-phenyl-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4gdg)**

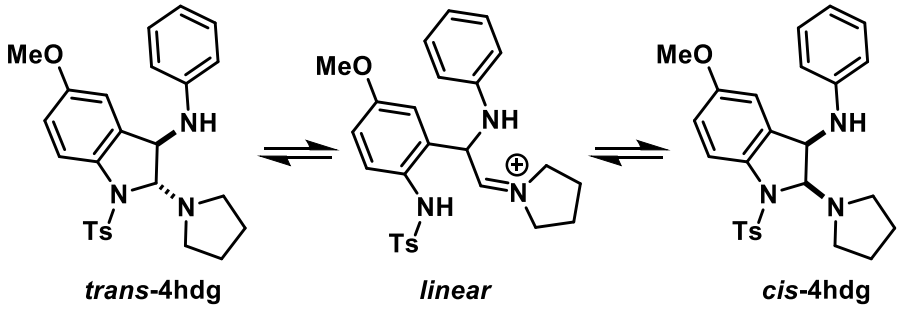


trans*-4gdg** ***linear ***cis*-4gdg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure B using 285 mg (1.0 mmol) of **S1g** and 0.091 mL (1.0 mmol) of **2d**. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4gdg** (171 mg, 0.38 mmol, 38% yield) as a beige solid.

Beige solid (171 mg, 0.38 mmol, 38% yield; mp 127–129 °C, dec.); IR (KBr) ν: 3406, 3051, 3026, 2970, 2922, 2856, 2839, 2806, 1348, 1165, 752, 696 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, J = 8.4 Hz, 1H), 7.40 (d, J = 8.4 Hz, 2H), 7.20 (t, J = 7.2 Hz, 2H), 7.18 (d, J = 8.4 Hz, 1H), 7.09 (d, J = 8.4 Hz, 2H), 7.00 (s, 1H), 6.76 (t, J = 7.5 Hz, 1H), 6.41 (d, J = 7.8 Hz, 2H), 5.11 (s, 1H), 4.45 (d, J = 7.2 Hz, 1H), 2.76–2.79 (m, 2H), 2.53–2.57 (m, 2H), 2.39 (s, 3H), 2.31 (s, 3H), 1.73–1.75 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 145.7, 143.6, 140.3, 135.18, 135.15, 132.5, 131.0, 129.5, 129.4, 127.4, 126.0, 118.1, 117.5, 113.2, 85.7, 59.9, 47.5, 23.5, 21.7, 21.2; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{26}H_{29}N_3O_2SNa$ 470.1878; Found 470.1882.

***trans*-5-Methoxy-*N*-phenyl-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4hdg)**



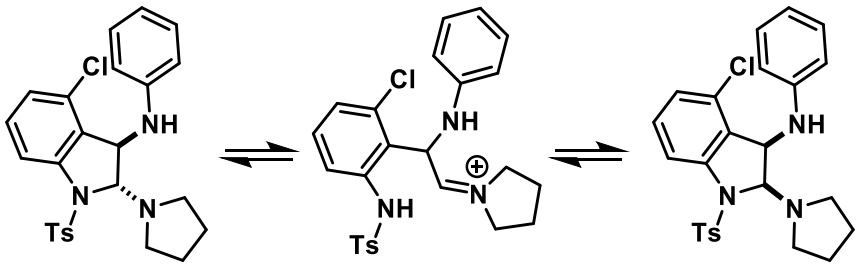
trans*-4hdg** ***linear ***cis*-4hdg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 499 mg (1.0 mmol) of **1h** and 0.091 mL (1.0 mmol) of **2d** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4hdg** (312 mg, 0.67 mmol, 67% yield) as a pale beige solid.

Pale beige solid (312 mg, 0.67 mmol, 67% yield; mp 129–131 °C, dec.); IR (KBr) ν: 3408, 3049, 3026, 2970, 2870, 2833, 2798, 1348, 1228, 1167, 1034, 750, 696 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.64 (d, J = 9.0 Hz, 1H), 7.38 (d, J = 7.8 Hz, 2H), 7.19 (t, J = 7.5 Hz, 2H), 7.10 (d, J = 7.8 Hz, 2H), 6.93 (dd, J = 8.7, 2.7 Hz, 1H), 6.76 (t, J = 7.5 Hz, 1H), 6.73 (d, J = 3.0 Hz, 1H), 6.39 (d, J = 7.8 Hz, 2H), 5.08 (s, 1H), 4.44 (d, J = 7.8 Hz, 1H), 3.77 (s, 3H), 2.76–2.78 (m, 2H), 2.55–2.57 (m, 2H), 2.40 (s, 3H), 1.72–1.77 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz,

$CDCl_3$) δ 157.7, 145.6, 143.6, 136.0, 135.0, 133.9, 129.5, 129.4, 127.4, 118.9, 118.2, 116.0, 113.3, 110.4, 85.8, 60.1, 55.7, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{26}H_{29}N_3O_3SNa$ 486.1827; Found 486.1827.

***trans*-4-Chloro-*N*-phenyl-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4idg)**

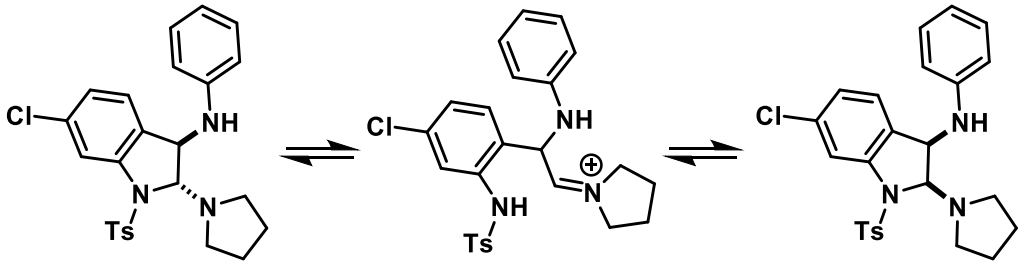


(*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure B using 306 mg (1.0 mmol) of **S1i** and 0.091 mL (1.0 mmol) of **2d**. The residue was purified by silica-gel column chromatography using hexane/AcOEt (20/1–8/1 [v/v]) and recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4idg** (212 mg, 0.45 mmol, 45% yield) as a pale beige solid.

Pale beige solid (212 mg, 0.45 mmol, 45% yield; mp 134–136 °C, dec.); IR (KBr) ν: 3406, 3095, 3047, 3030, 2970, 2927, 2875, 2856, 2804, 1356, 1169, 760, 704 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, J = 8.4 Hz, 1H), 7.45 (d, J = 8.4 Hz, 2H), 7.32 (t, J = 7.8 Hz, 1H), 7.22 (t, J = 8.1 Hz, 2H), 7.11 (d, J = 8.4 Hz, 2H), 7.08 (d, J = 7.8 Hz, 1H), 6.79 (t, J = 7.2 Hz, 1H), 6.47 (d, J = 7.2 Hz, 2H), 5.22 (s, 1H), 4.60 (d, J = 6.0 Hz, 1H), 2.76–2.79 (m, 2H), 2.53–2.56 (m, 2H), 2.40 (s, 3H), 1.74–1.79 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 145.7, 144.05, 144.05, 135.0, 131.6, 131.4, 130.2, 129.6, 129.4, 127.5, 125.5, 118.3, 115.8, 113.3, 86.0, 59.2, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}ClN_3O_2SNa$ 490.1332, 492.1302; Found 490.1335, 492.1301.

***trans*-6-Chloro-*N*-phenyl-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4jdg)**



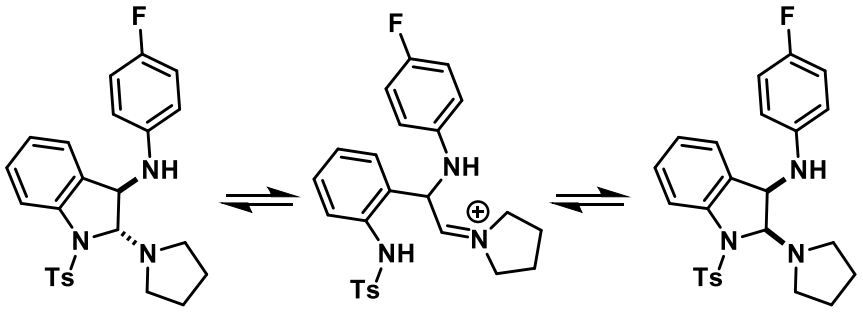
(*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1j** and 0.091 mL (1.0 mmol) of **2d** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4jdg** (375 mg, 0.80 mmol, 80% yield) as a pale beige solid.

Pale beige solid (375 mg, 0.80 mmol, 80% yield; mp 127–129 °C, dec.); IR (KBr) ν: 3406, 3101, 3066, 3028, 2970, 2925, 2871, 2850, 1352, 1165, 758, 702 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 1.8 Hz, 1H), 7.44 (d, J = 7.8 Hz, 2H), 7.21 (t, J = 7.2 Hz, 2H), 7.12–7.14 (m, 3H), 7.08 (dd, J = 7.8, 1.8 Hz, 1H), 6.78 (t, J =

7.2 Hz, 1H), 6.41 (d, J = 7.2 Hz, 2H), 5.17 (s, 1H), 4.47 (d, J = 7.8 Hz, 1H), 2.76–2.79 (m, 2H), 2.54–2.57 (m, 2H), 2.41 (s, 3H), 2.39 (d, J = 7.2 Hz, 1H), 1.74–1.79 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 145.4, 144.1, 143.8, 136.0, 135.0, 130.9, 129.7, 129.5, 127.4, 126.4, 125.5, 118.5, 118.0, 113.3, 86.4, 59.3, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}ClN_3O_2SNa$ 490.1332, 492.1302; Found 490.1331, 492.1306.

***trans*-*N*-(4-Fluorophenyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4ajg)**

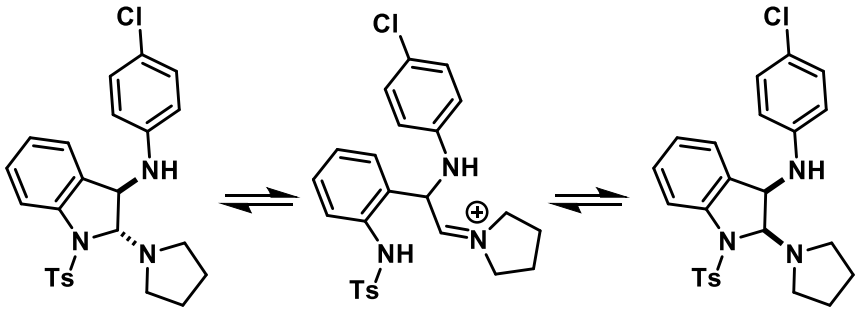


trans*-4ajg** ***linear ***cis*-4ajg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.096 mL (1.0 mmol) of **2j** for 2 h. The residue was purified by recrystallization using hexane/ethanol (2/1 [v/v]) to give *trans*-**4ajg** (365 mg, 0.81 mmol, 81% yield) as a white solid.

White solid (365 mg, 0.81 mmol, 81% yield; mp 139–141 °C, dec.); IR (KBr) ν: 3415, 3028, 2960, 2924, 2866, 1350, 1167, 764, 708 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, J = 8.4 Hz, 1H), 7.40 (d, J = 7.8 Hz, 2H), 7.38 (td, J = 8.7, 1.5 Hz, 1H), 7.20 (dd, J = 7.8, 0.6 Hz, 1H), 7.12 (td, J = 8.4, 0.9 Hz, 1H), 7.08 (d, J = 7.8 Hz, 2H), 6.91 (t, J = 8.7 Hz, 2H), 6.33–6.37 (m, 2H), 5.10 (s, 1H), 4.43 (d, J = 7.2 Hz, 1H), 2.76–2.79 (m, 2H), 2.53–2.56 (m, 2H), 2.38 (s, 3H), 2.30 (d, J = 7.2 Hz, 1H), 1.71–1.76 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 156.2 (d, J_{C-F} = 235.7 Hz), 143.8, 142.6, 141.9, 135.1, 132.3, 130.3, 129.5, 127.4, 125.4 (d, J_{C-F} = 17.4 Hz), 117.8, 116.0, 115.8, 114.0 (d, J_{C-F} = 7.2 Hz), 85.3, 60.3, 47.4, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}FN_3O_2SNa$ 474.1627; Found 474.1632.

***trans*-*N*-(4-Chlorophenyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4akg)**

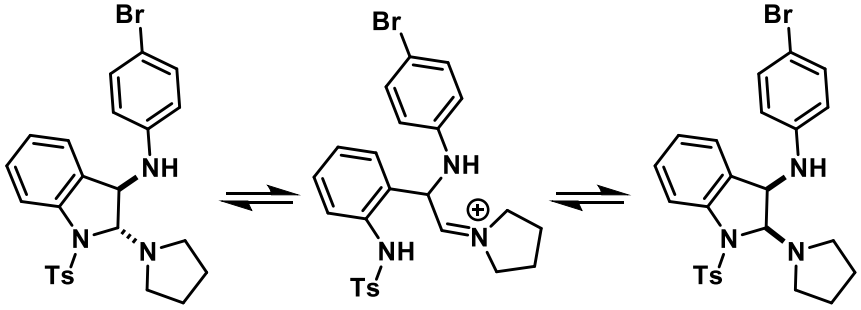


trans*-4akg** ***linear ***cis*-4akg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 128 mg (1.0 mmol) of **2k** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4akg** (410 mg, 0.88 mmol, 88%yield) as a white solid.

White solid (410 mg, 0.88 mmol, 88% yield; mp 154–156 °C, dec.); IR (KBr) ν: 3402, 3068, 3026, 2972, 2918, 2856, 1350, 1168, 758, 706 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 7.8 Hz, 1H), 7.37–7.41 (m, 3H), 7.20 (d, J = 7.2 Hz, 1H), 7.15 (d, J = 9.0 Hz, 2H), 7.12 (td, J = 6.9, 1.2 Hz, 1H), 7.08 (d, J = 7.8 Hz, 2H), 6.33 (d, J = 8.4 Hz, 2H), 5.08 (s, 1H), 4.44 (d, J = 7.2 Hz, 1H), 2.75–2.78 (m, 2H) 2.53–2.55 (m, 2H), 2.39 (d, J = 7.2 Hz, 1H), 2.38 (s, 3H), 1.72–1.76 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 144.2, 143.8, 142.7, 135.1, 132.1, 130.5, 129.5, 129.3, 127.3, 125.51, 125.46, 122.8, 117.9, 114.3, 85.2, 59.9, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}ClN_3O_2SNa$ 490.1332, 492.1302; Found 490.1328, 492.1305.

***trans*-*N*-(4-Bromophenyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4alg)**

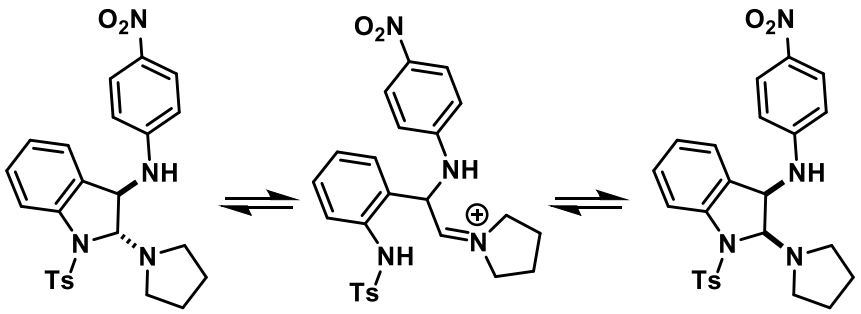


(*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 172 mg (1.0 mmol) of **2l** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4alg** (447 mg, 0.87 mmol, 87% yield) as a white solid.

White solid (447 mg, 0.87 mmol, 87% yield; mp 151–153 °C, dec.); IR (KBr) ν: 3402, 3070, 3022, 2970, 2918, 2856, 1350, 1169, 758, 706 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 7.8 Hz, 1H), 7.39 (td, J = 8.4, 1.5 Hz, 1H), 7.38 (d, J = 8.4 Hz, 2H), 7.28 (d, J = 9.0 Hz, 2H), 7.20 (d, J = 7.2 Hz, 1H), 7.12 (td, J = 8.4, 0.9 Hz, 1H), 7.08 (d, J = 7.8 Hz, 2H), 6.29 (d, J = 8.4 Hz, 2H), 5.07 (s, 1H), 4.43 (d, J = 7.2 Hz, 1H), 2.75–2.78 (m, 2H), 2.52–2.55 (m, 2H), 2.41 (d, J = 7.2 Hz, 1H), 2.38 (s, 3H), 1.71–1.78 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 144.6, 143.8, 142.7, 135.1, 132.1, 132.0, 130.4, 129.5, 127.3, 125.51, 125.47, 117.9, 114.9, 109.9, 85.3, 59.9, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}BrN_3O_2SNa$ 534.0827, 536.0806; Found 534.0827, 536.0809.

***trans*-*N*-(4-Nitrophenyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4amg)**

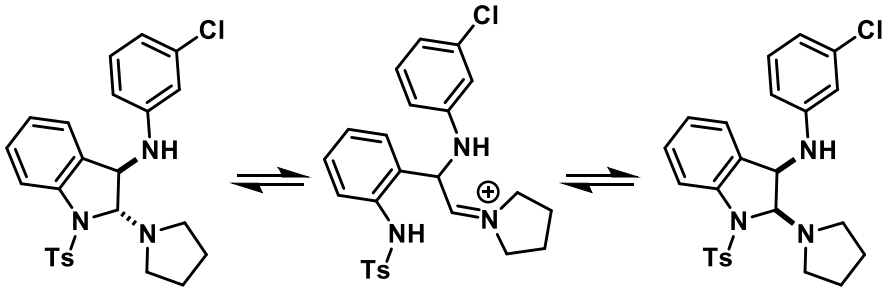


(*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 138 mg (1.0 mmol) of **2m** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4amg** (256 mg, 0.53 mmol, 53% yield) as a pale green solid.

Pale green solid (256 mg, 0.53 mmol, 53% yield; mp 139–141 °C, dec.); IR (KBr) ν: 3340, 3078, 2968, 2920, 2879, 2841, 1518, 1352, 1311, 1171, 752, 706 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, J = 9.0 Hz, 2H), 7.78 (d, J = 8.4 Hz, 1H), 7.45 (td, J = 8.4, 1.2 Hz, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.23 (dd, J = 7.8, 0.6 Hz, 1H), 7.17 (td, J = 8.4, 0.9 Hz, 1H), 7.09 (d, J = 8.4 Hz, 2H), 6.36 (d, J = 9.0 Hz, 2H), 5.06 (s, 1H), 4.53 (d, J = 6.6 Hz, 1H), 3.07 (d, J = 6.6 Hz, 1H), 2.77–2.80 (m, 2H), 2.54–2.57 (m, 2H), 2.40 (s, 3H), 1.74–1.79 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 150.7, 144.0, 142.9, 139.1, 135.0, 131.0, 130.8, 129.7, 127.3, 126.4, 125.8, 125.5, 118.3, 112.0, 85.3, 59.9, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}N_4O_4SNa$ 501.1572; Found 501.1572.

***trans*-*N*-(3-Chlorophenyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4ang)**

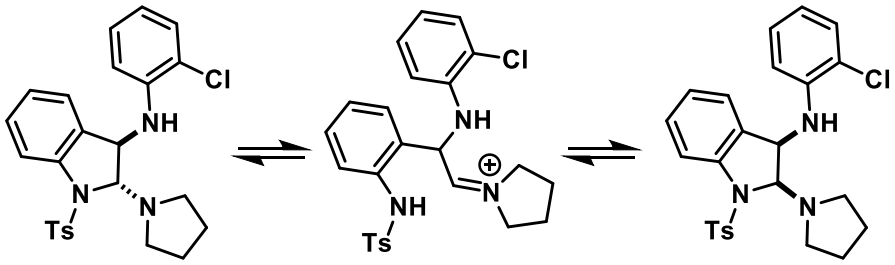


(*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.105 mL (1.0 mmol) of **2n** for 1 h. The residue was purified by recrystallization using hexane/ethanol (2/1 [v/v]) and silica-gel column chromatography using hexane/AcOEt (10/1–8/1 [v/v]) to give *trans*-**4ang** (455 mg, 0.97 mmol, 97% yield) as a white solid.

White solid (455 mg, 0.97 mmol, 97% yield; mp 148–150 °C, dec.); IR (KBr) ν: 3427, 3095, 3024, 2964, 2922, 2870, 2844, 1348, 1169, 758, 708 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, J = 8.4 Hz, 1H), 7.40 (td, J = 7.8, 1.2 Hz, 1H), 7.38 (d, J = 8.4 Hz, 2H), 7.20 (d, J = 7.8 Hz, 1H), 7.09–7.15 (m, 4H), 6.72 (ddd, J = 8.1, 2.1, 0.6 Hz, 1H), 6.34 (dd, J = 8.1, 1.5 Hz, 1H), 6.25 (t, J = 2.1 Hz, 1H), 5.06 (s, 1H), 4.45 (d, J = 7.2 Hz, 1H), 2.75–2.79 (m, 2H), 2.52–2.56 (m, 2H), 2.41 (s, 3H), 2.39 (d, J = 7.2 Hz, 1H), 1.72–1.77 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 146.6, 144.0, 142.8, 135.1, 135.0, 132.0, 130.50, 130.47, 129.7, 127.3, 125.53, 125.48, 118.1, 118.0, 113.9, 110.9, 85.2, 59.8, 47.5, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{26}ClN_3O_2SNa$ 490.1332, 492.1302; Found 490.1333, 492.1305.

***trans*-*N*-(2-Chlorophenyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4aog)**

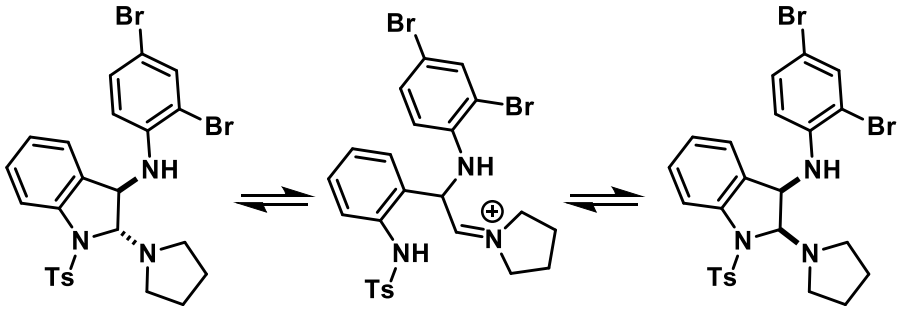


trans*-4aog** ***linear ***cis*-4aog** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.105 mL (1.0 mmol) of **2o** for 3 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4aog** (412 mg, 0.88 mmol, 88% yield) as a white solid.

White solid (412 mg, 0.88 mmol, 88% yield; mp 149–151 °C, dec.); IR (KBr) ν: 3419, 3032, 2972, 2918, 2871, 2843, 1350, 1165, 754, 706 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, J = 7.8 Hz, 1H), 7.42 (d, J = 8.4 Hz, 2H), 7.39 (td, J = 8.1, 0.9 Hz, 1H), 7.19–7.24 (m, 3H), 7.13 (t, J = 7.5 Hz, 1H), 7.05 (d, J = 8.4 Hz, 1H), 6.99 (d, J = 7.2 Hz, 1H), 6.72 (td, J = 8.7, 1.2 Hz, 1H), 5.22 (s, 1H), 4.49 (d, J = 6.0 Hz, 1H), 3.36 (d, J = 6.0 Hz, 1H), 2.80–2.83 (m, 2H), 2.57–2.61 (m, 2H), 2.32 (s, 3H), 1.74–1.79 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 144.2, 142.8, 142.0, 134.8, 131.6, 130.5, 129.7, 129.4, 128.2, 127.2, 125.6, 125.4, 118.9, 118.2, 117.4, 112.3, 85.7, 60.3, 47.4, 23.5, 21.8; HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{25}H_{27}ClN_3O_2S$ 468.1513, 470.1483; Found 468.1516, 470.1478.

***trans*-*N*-(2,4-Dibromophenyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4apg)**



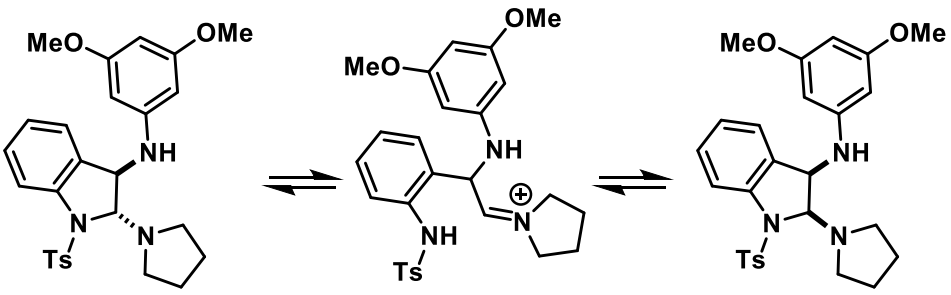
trans*-4apg** ***linear ***cis*-4apg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 251 mg (1.0 mmol) of **2p** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4apg** (371 mg, 0.63 mmol, 63% yield) as a white solid.

White solid (371 mg, 0.63 mmol, 63% yield; mp 152–154 °C, dec.); IR (KBr) ν: 3398, 3032, 2970, 2912, 2841, 1354, 1171, 756, 704 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 2.4 Hz, 1H), 7.41 (d, J = 7.8 Hz, 2H), 7.39 (td, J = 8.4, 1.2 Hz, 1H), 7.37 (dd, J = 8.7, 2.1 Hz, 1H), 7.24 (d, J = 7.2 Hz, 1H), 7.14 (td, J = 7.8, 0.9 Hz, 1H), 7.06 (d, J = 8.4 Hz, 2H), 6.88 (d, J = 8.4 Hz, 1H), 5.17 (s, 1H), 4.43 (d, J = 5.4 Hz, 1H), 3.41 (d, J = 5.4 Hz, 1H), 2.79–2.82 (m, 2H), 2.56–2.60 (m, 2H), 2.32 (s, 3H), 1.73–1.81 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 144.2, 142.8, 142.2, 134.8, 134.6, 131.8, 131.1, 130.6, 129.8, 127.2, 125.48,

125.45, 117.5, 113.5, 109.6, 109.3, 85.5, 60.6, 47.4, 23.5, 21.9; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{25}Br_2N_3O_2SNa$ 611.9932; Found 611.9932.

***trans*-*N*-(3,5-Dimethoxyphenyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4aqg)**

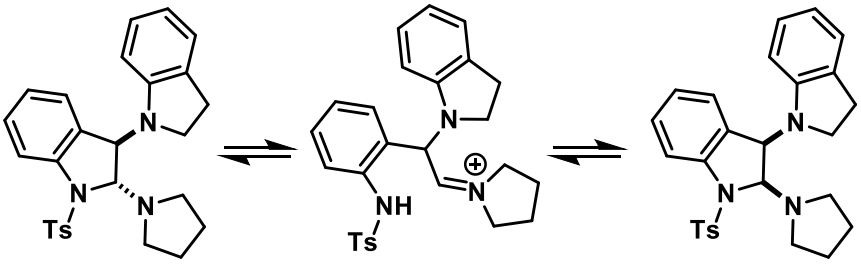


(*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 153 mg (1.0 mmol) of **2q** for 3 h. The residue was purified by recrystallization using hexane/ethanol (2/1 [v/v]) and silica-gel column chromatography using hexane/AcOEt (6/1–4/1 [v/v]) to give *trans*-**4aqg** (282 mg, 0.57 mmol, 57% yield) as a white solid.

White solid (282 mg, 0.57 mmol, 57% yield; mp 139–141 °C, dec.); IR (KBr) ν: 3413, 2958, 2933, 2875, 2839, 1348, 1248, 1168, 1066, 754 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, J = 8.4 Hz, 1H), 7.41 (d, J = 8.4 Hz, 2H), 7.37 (td, J = 8.4, 1.2 Hz, 1H), 7.20 (d, J = 7.2 Hz, 1H), 7.10–7.12 (m, 3H), 5.94 (t, J = 2.1 Hz, 1H), 5.69 (d, J = 1.8 Hz, 2H), 5.19 (s, 1H), 4.48 (d, J = 7.2 Hz, 1H), 3.77 (s, 6H), 2.76–2.81 (m, 2H), 2.55–2.59 (m, 2H), 2.49 (d, J = 7.2 Hz, 1H), 2.37 (s, 3H), 1.69–1.76 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 161.8, 147.6, 143.7, 142.7, 135.0, 132.2, 130.3, 129.5, 127.4, 125.6, 125.4, 117.8, 92.2, 90.7, 85.8, 60.0, 55.3, 47.4, 23.5, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{27}H_{31}N_3O_4SNa$ 156.1933; Found 156.1930.

***trans*-2'-(Pyrrolidin-1-yl)-1'-tosyl-1,3'-biindoline (4afg)**



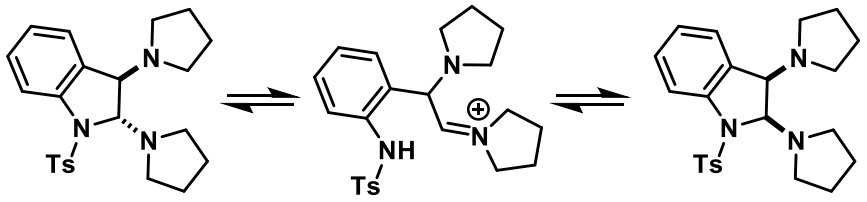
(*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.111 mL (1.0 mmol) of **2f** for 2 h. The residue was purified by recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4afg** (413 mg, 0.90 mmol, 90% yield) as a white solid.

White solid (413 mg, 0.90 mmol, 90% yield; mp 141–143 °C, dec.); IR (KBr) ν: 2976, 2943, 2902, 2868, 2837, 2738, 2677, 1338, 1169, 758, 708 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.71 (d, J = 8.4 Hz, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.35 (td, J = 8.4, 1.2 Hz, 1H), 7.14 (t, J = 6.9 Hz, 1H), 7.11 (d, J = 9.6 Hz, 1H), 7.09 (d, J = 8.4 Hz,

2H), 7.05 (td, *J* = 8.4, 1.5 Hz, 1H), 7.03 (d, *J* = 7.2 Hz, 1H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.70 (td, *J* = 7.8, 0.9 Hz, 1H), 5.33 (d, J = 1.2 Hz, 1H), 4.48 (s, 1H), 2.79–2.83 (m, 2H), 2.69 (q, *J* = 9.6 Hz, 1H), 2.56–2.63 (m, 3H), 2.33 (s, 3H), 1.72–1.77 (m, 4H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 151.2, 143.6, 142.9, 136.1, 130.2, 130.0, 129.30, 129.27, 127.7, 127.6, 126.8, 124.5, 124.2, 118.2, 116.7, 107.5, 85.7, 63.5, 49.4, 47.3, 28.3, 23.6, 21.6; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{27}H_{29}N_3O_2SNa$ 482.1878; Found 482.1883.

***trans*-2,3-Di(pyrrolidin-1-yl)-1-tosylindoline (4agg)**

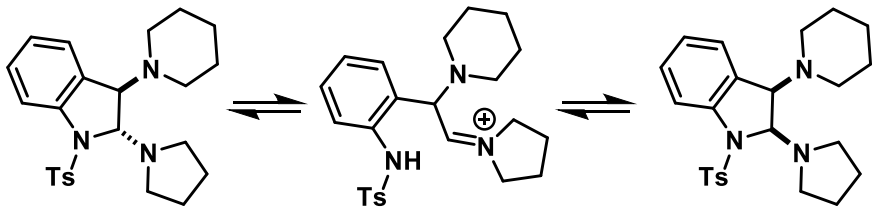


trans*-4agg** ***linear ***cis*-4agg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.083 mL (1.0 mmol) of **2g** for 2 h. The residue was purified by silica-gel column chromatography using hexane/AcOEt (3/1–1/1 [v/v]) and recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4agg** (366 mg, 0.90 mmol, 90% yield) as a beige solid.

Beige solid (366 mg, 0.90 mmol, 90% yield; mp 98–100 °C, dec.); IR (KBr) ν: 3066, 3035, 2966, 2925, 2873, 2819, 2796, 1352, 1167, 756, 704 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.8 Hz, 2H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.24 (td, *J* = 8.4, 1.2 Hz, 1H), 7.14 (d, *J* = 7.2 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 2H), 6.99 (td, *J* = 8.7, 0.9 Hz, 1H), 5.22 (s, 1H), 3.45 (s, 1H), 2.69–2.72 (m, 2H), 2.41–2.47 (m, 4H), 2.28 (s, 3H), 2.11–2.14 (m, 2H), 1.63–1.67 (m, 4H), 1.49–1.52 (m, 2H), 1.38–1.42 (m, 2H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 143.2, 142.6, 136.0, 132.0, 129.2, 128.8, 127.7, 126.7, 123.8, 116.6, 84.7, 69.3, 51.0, 47.5, 23.2, 23.0, 21.5; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{29}N_3O_2SNa$ 434.1878; Found 434.1877.

***trans*-3-(Piperidin-1-yl)-2-(pyrrolidin-1-yl)-1-tosylindoline (4ahg)**



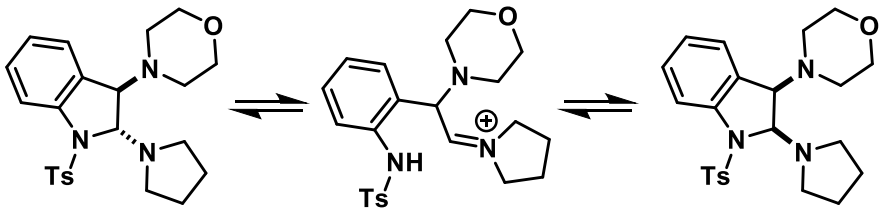
trans*-4ahg** ***linear ***cis*-4ahg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.099 mL (1.0 mmol) of **2h** for 6 h. The residue was purified by silica-gel column chromatography using hexane/AcOEt (6/1–1/1 [v/v]) and methanol and recrystallization using hexane/isopropanol (2/1 [v/v]) to give *trans*-**4ahg** (421 mg, 0.99 mmol, 99% yield) as a pale beige solid.

Pale beige solid (421 mg, 0.99 mmol, 99% yield; mp 102–104 °C, dec.); IR (KBr) ν: 3066, 3032, 2964, 2937, 2873, 2848, 2800, 2740, 1352, 1167, 752, 706 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.8 Hz, 2H),

7.56 (d, J = 7.8 Hz, 1H), 7.23 (t, J = 7.8 Hz, 1H), 7.16 (d, J = 7.8 Hz, 1H), 7.11 (d, J = 9.0 Hz, 2H), 6.98 (t, J = 7.5 Hz, 1H), 5.29 (s, 1H), 3.60 (s, 1H), 2.71–2.74 (m, 2H), 2.47–2.51 (m, 2H), 2.29 (s, 3H), 2.15–2.18 (m, 2H), 2.05-2.06 (m, 2H), 1.59–1.68 (m, 4H), 1.29 (br s, 4H), 1.22–1.23 (m, 2H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 143.6, 142.7, 136.4, 130.3, 129.4, 129.2, 127.9, 127.3, 123.5, 115.8, 83.3, 71.1, 51.1, 47.3, 26.1, 24.6, 23.4, 21.6; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{24}H_{31}N_3O_2SNa$ 448.2035; Found 448.2037.

4-(*trans*-2-(Pyrrolidin-1-yl)-1-tosylindolin-3-yl)morpholine (4aig)

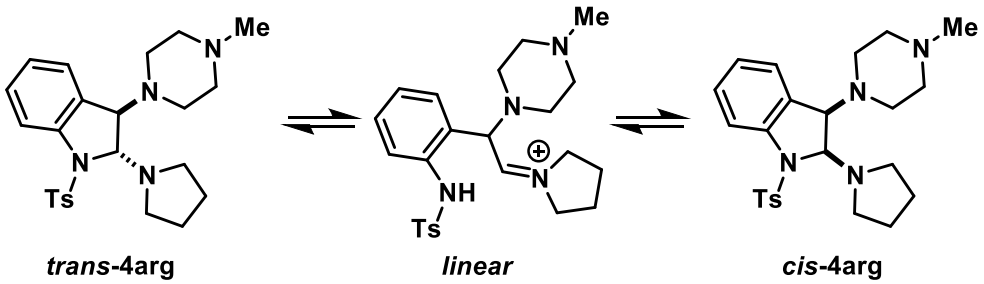


trans*-4aig** ***linear ***cis*-4aig** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.087 mL (1.0 mmol) of **2i** for 6 h. The residue was purified by silica-gel column chromatography using hexane/AcOEt (6/1–1/6 [v/v]) and methanol to give *trans*-**4aig** (411 mg, 0.96 mmol, 96% yield) as brown oil.

Brown oil (411 mg, 0.96 mmol, 96% yield); IR (KBr) ν: 3064, 3030, 2958, 2854, 2763, 2690, 1354, 1165, 756, 706 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.68 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 8.4 Hz, 1H), 7.29 (td, J = 8.4, 1.2 Hz, 1H), 7.13-7.16 (m, 3H), 7.02 (td, J = 7.5, 0.6 Hz, 1H), 5.24 (s, 1H), 3.54 (s, 1H), 3.41-3.44 (m, 2H), 3.30–3.31 (m, 2H), 2.73–2.74 (m, 2H), 2.49–2.50 (m, 2H), 2.32 (s, 3H), 2.29–2.31 (m, 2H), 2.10–2.13 (m, 2H), 1.66–1.69 (m, 4H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 143.4, 142.6, 136.0, 129.5, 129.12, 129.07, 127.6, 127.2, 123.6, 116.2, 83.2, 70.5, 66.6, 50.3, 47.2, 23.1, 21.3; HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{23}H_{30}N_3O_3S$ 428.2008; Found 428.2013.

***trans*-3-(4-Methylpiperazin-1-yl)-2-(pyrrolidin-1-yl)-1-tosylindoline (4arg)**



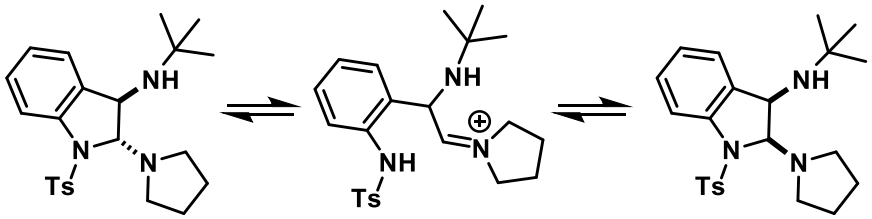
trans*-4arg** ***linear ***cis*-4arg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.110 mL (1.0 mmol) of **2r** for 6 h. The residue was purified by silica-gel column chromatography using chloroform/methanol (10/1–8/1 [v/v]) and recrystallization using hexane/diethyl ether (2/1 [v/v]) to give *trans*-**4arg** (146 mg, 0.33 mmol, 33% yield) as a pale beige solid.

Pale beige solid (146 mg, 0.33 mmol, 33% yield; mp 120–122 °C, dec.); IR (KBr) ν: 3068, 3033, 2966, 2933, 2877, 2839, 2798, 2746, 2686, 1342, 1167, 752, 704 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (d, J = 8.4 Hz,

2H), 7.59 (d, J = 8.4 Hz, 1H), 7.24 (td, J = 8.7, 1.2 Hz, 1H), 7.13 (d, J = 7.2 Hz, 1H), 710 (d, J = 7.8 Hz, 2H), 6.99 (td, J = 7.2, 0.9 Hz, 1H), 5.22 (d, J = 0.6 Hz, 1H), 3.54 (s, 1H), 2.69–2.72 (m, 2H), 2.45–2.49 (m, 2H), 2.29 (br s, 5H), 2.14–2.17 (m, 6H), 1.60–1.68 (m, 4H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 143.3, 142.7, 136.2, 129.8, 129.5, 129.3, 127.8, 127.3, 123.6, 116.2, 83.5, 70.4, 54.9, 49.6, 47.3, 45.9, 23.3, 21.5; HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{24}H_{33}N_4O_2S$ 441.2324; Found 441.2323.

***trans*-*N*-(*tert*-Butyl)-2-(pyrrolidin-1-yl)-1-tosylindolin-3-amine (4abg)**

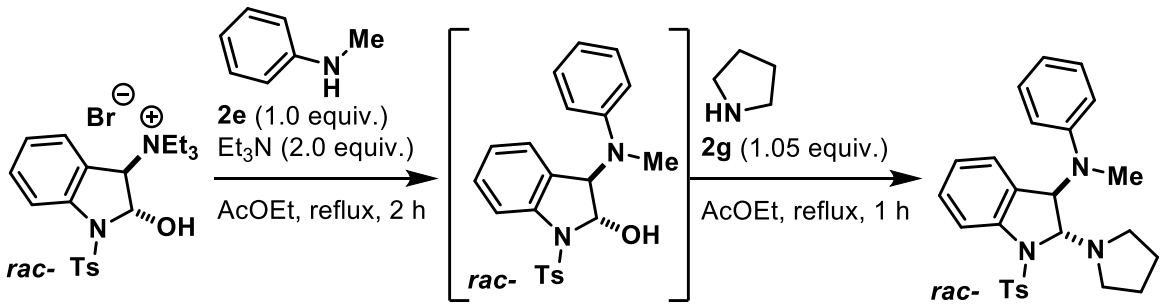


trans*-4abg** ⇌ ***linear ⇌ ***cis*-4abg** (*trans*:*cis* = >20:<1)

The reaction was performed according to the general procedure A using 469 mg (1.0 mmol) of **1a** and 0.106 mL (1.0 mmol) of **2b** for 2 h. The residue was purified by silica-gel column chromatography using hexane/AcOEt (10/1–8/1 [v/v]) to give *trans*-**4abg** (7.1 mg, 0.02 mmol, trace) as a dark red oil.

Dark red oil (7.1 mg, 0.02 mmol, trace); IR (KBr) ν: 3338, 3066, 2964, 2931, 2873, 1354, 1167, 754, 708 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58–7.61 (m, 3H), 7.24 (td, J = 8.7, 1.2 Hz, 1H), 7.12 (d, J = 9.0 Hz, 2H), 7.04–7.08 (m, 2H), 5.01 (s, 1H), 3.89 (s, 1H), 2.70–2.74 (m, 2H), 2.46–2.49 (m, 2H), 2.30 (s, 3H), 1.64–1.69 (m, 4H), 1.02 (s, 9H), 0.97 (s, 1H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 143.6, 142.0, 135.7, 135.3, 129.3, 129.1, 128.0, 125.11, 125.05, 117.1, 90.1, 59.6, 51.4, 47.7, 29.9, 23.4, 21.6; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{31}N_3O_2SNa$ 436.2035; Found 436.2034.

Scheme S5 Gram-scale synthesis of 2,3-diaminoindolines



trans-**1a**
9.39 g (20 mmol)

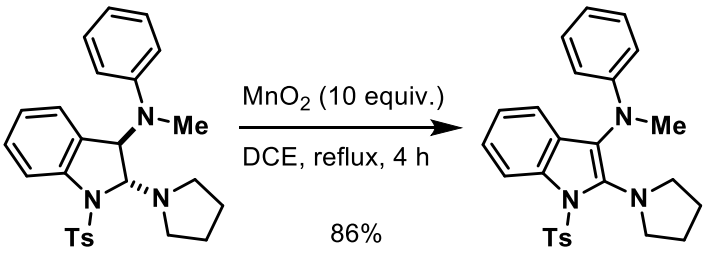
trans-**3aeg**

trans-**4aeg**
8.78 g, 98%

To a suspension of *trans*-**1a** (9.39 g, 20 mmol) and **2e** (2.16 mL, 1.0 equiv., 20 mmol) in AcOEt (100 mL, 0.2 M) was added Et_3N (5.54 mL, 2.0 equiv., 40 mmol). The suspension was stirred at reflux in an oil bath for 2 h. Then **2g** (1.74 mL, 1.05 equiv., 21 mmol) was added to the mixture and stirred for a further 1 h. After the whole was cooled to room temperature, the resulting mixture was concentrated *in vacuo*. The residue was purified by recrystallization using (EtOH/hexane) to give *trans*-**4aeg** (8.78 g, 19.6 mmol, 98%) as a white solid.

Scheme S6 Follow up chemistry

***N*-Methyl-*N*-phenyl-2-(pyrrolidin-1-yl)-1-tosyl-*1H*-indol-3-amine (5aeg)**

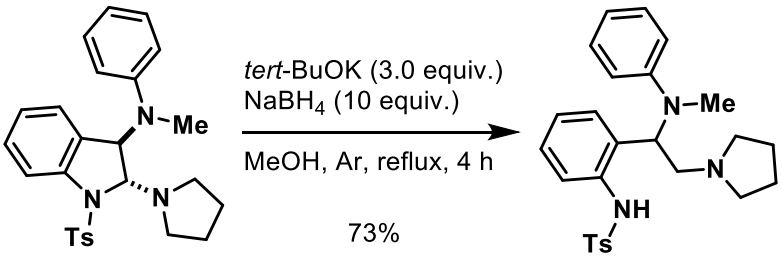


trans-**4aeg** **5aeg**

To a mixture of *trans*-**4aeg** (448 mg, 1.0 mmol) and MnO_2 (869 mg, 10 equiv., 10 mmol) was added DCE (5.0 mL, 0.2 M). The suspension was stirred at reflux in oil bath for 4 h. After the whole was cooled to room temperature, the mixture was filtered through a celite pad. The resulting filtrate was concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt (10/1 v/v) to give **5aeg** (384 mg, 0.86 mmol, 86% yield) as a white solid.

White solid (384 mg, 0.86 mmol, 86% yield; mp 153–155 °C); IR (KBr) ν: 3062, 3026, 2972, 2929, 2871, 1363, 1173, 754 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 8.20 (d, J = 8.4 Hz, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.24 (td, J = 7.8, 1.2 Hz, 1H), 7.19 (d, J = 7.8 H, 2H), 7.14 (td, J = 7.8, 0.6 Hz, 1H), 7.09 (t, J = 7.8 Hz, 2H), 6.87 (d, J = 7.8 Hz, 1H), 6.72 (t, J = 7.2 Hz, 1H), 6.33 (d, J = 7.8 Hz, 2H), 3.23 (br s, 4H), 3.12 (s, 3H), 2.42 (s, 3H), 1.87–1.85 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 148.2, 144.4, 142.9, 134.7, 134.1, 129.9, 129.2, 128.9, 127.1, 124.5, 123.4, 117.8, 117.7, 117.1, 117.0, 112.5, 50.9, 39.9, 25.2, 21.7; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{26}H_{27}N_3O_2SNa$ 468.1722; Found 468.1725.

4-Methyl-*N*-(2-(1-(methyl(phenyl)amino)-2-(pyrrolidin-1-yl)ethyl)phenyl)benzenesulfonamide (6)



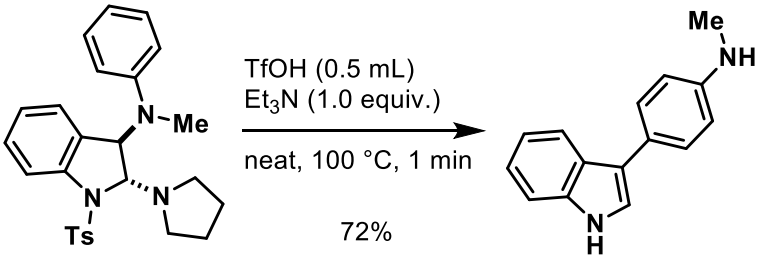
trans-**4aeg** **6**

To a mixture of *trans*-**4aeg** (224 mg, 0.50 mmol) and *tert*-BuOK (168 mg, 3.0 equiv., 1.5 mmol) in MeOH (2.5 mL, 0.20 M) was added $NaBH_4$ (189 mg, 10 equiv., 5.0 mmol) under Ar atmosphere. The suspension was stirred at reflux in oil bath for 4 h. After the whole was cooled to room temperature, H_2O (20 mL) was added to the mixture. The whole was extracted with AcOEt (3 x 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by recrystallization using methanol to give **6** (165 mg, 0.73 mmol, 73% yield) as a white solid.

White solid (165 mg, 0.73 mmol, 73% yield; mp 119–121 °C); IR (KBr) ν: 3057, 2951, 2897, 2875, 2831, 2509,

1333, 1159, 1092, 756 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 13.99 (br s,1H) 7.73 (d, J = 7.8 Hz, 1H), 7.70 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 7.8 Hz, 2H), 7.20 (td, J = 8.4, 1.5 Hz, 1H), 7.03 (t, J = 7.8 Hz, 2H), 6.94 (t, J = 7.2 Hz, 1H), 6.90 (d, J = 6.6 Hz, 1H), 6.66 (t, J = 7.5 Hz, 1H), 6.19 (d, J = 7.8 Hz, 2H), 4.61 (d, J = 8.4 Hz, 1H), 3.26 (dd, J = 12.3, 1.2 Hz, 1H), 2.94 (s, 3H), 2.90 (d, J = 12.0 Hz, 1H), 2.84–2.85 (m, 2H), 2.62 (br s, 2H), 2.43 (s, 3H), 1.95–2.03 (m, 4H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 148.7, 143.0, 139.0, 136.8, 134.3, 129.8, 129.1, 128.1, 126.8, 126.7, 124.4, 123.1, 116.9, 112.2, 62.3, 58.2, 54.1, 35.0, 23.8, 21.8; HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{32}N_3O_2S$ 450.2215; Found 450.2217.

4-(1*H*-Indol-3-yl)-*N*-methylaniline (7)

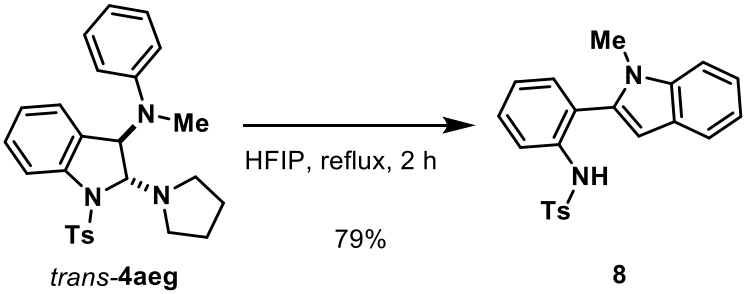


trans-**4aeg** **7**

trans-**4aeg** (44.7 mg, 0.10 mmol) and Et_3N (10.7 mg, 1.0 equiv., 0.10 mmol) were stirred at 100 °C in oil bath under solvent-free condition. Then, TfOH (0.5 mL) was added to the mixture and stirred for 1 minute. After the whole was cooled down to room temperature, the mixture was quenched with sat. $NaHCO_3$ (5 mL) and extracted with AcOEt (3 x 10 mL). The combined organic layer was washed with brine (10 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt (1/1–0/1 v/v) to give **7** (15.9 mg, 0.072 mmol, 72%) as a pale-yellow oil.

Pale-yellow oil (15.9 mg, 0.072 mmol, 72%); IR (KBr) ν: 3357, 3153, 3099, 3055, 2916, 2858, 2816, 1506, 1246, 748 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 8.13 (br s, 1H), 7.91 (d, J = 8.4 Hz, 1H), 7.51 (d, J = 9.0 Hz, 2H), 7.41 (d, J = 7.8 Hz, 1H), 7.27 (d, J = 2.4 Hz, 1H), 7.23 (dt, J = 7.2, 1.2 Hz, 1H), 7.17 (dt, J = 7.8, 1.2 Hz, 1H), 6.74 (d, J = 9.0 Hz, 2H), 3.79 (br s, 1H), 2.90 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 147.9, 136.7, 128.7, 126.2, 124.8, 122.3, 120.8, 120.06, 120.06, 118.8, 113.0, 111.4, 31.1; HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{15}N_2$ 223.1235; Found 223.1242.

4-Methyl-*N*-(2-(1-methyl-*1H*-indol-2-yl)phenyl)benzenesulfonamide (8) [2c]

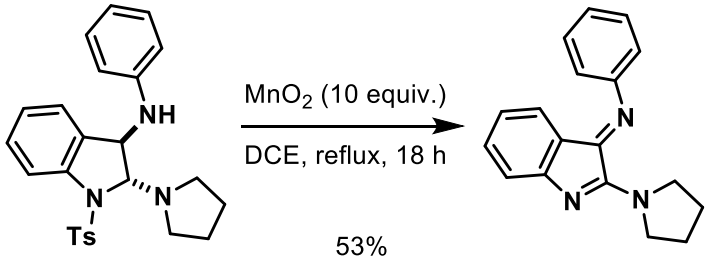


trans-**4aeg** **8**

A solution of *trans*-**4aeg** (44.7 mg, 0.1 mmol) in HFIP (1.0 mL, 0.1 M) was stirred at reflux for 2 h. The resulting mixture was cooled to room temperature and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1 v/v) to give **8** (29.6 mg, 0.079 mmol, 79% yield) as a white solid.

White solid (29.6 mg, 0.079 mmol, 79% yield; mp 145–147 °C); IR (KBr) ν: 3261, 3097, 3068, 2981, 2939, 1477, 1335, 1163, 752 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, J = 8.4 Hz, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.44–7.41 (m, 1H), 7.35–7.31 (m, 2H), 7.22 (ddd, J = 7.8, 6.0, 1.8 Hz, 1H), 7.19 (d, J = 4.2 Hz, 2H), 7.17 (d, J = 7.8 Hz, 2H), 7.12 (br s, 1H), 6.24 (s, 1H), 3.24 (s, 3H), 2.41 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 144.0, 137.9, 136.3, 135.9, 134.7, 131.4, 130.0, 129.7, 127.7, 127.2, 124.4, 123.3, 122.5, 120.9, 120.6, 120.4, 109.8, 102.6, 30.3, 21.6; HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{20}N_2O_2SNa$ 399.1143; Found 399.1139.

_N_-Phenyl-2-(pyrrolidin-1-yl)-3_H_-indol-3-imine (9)



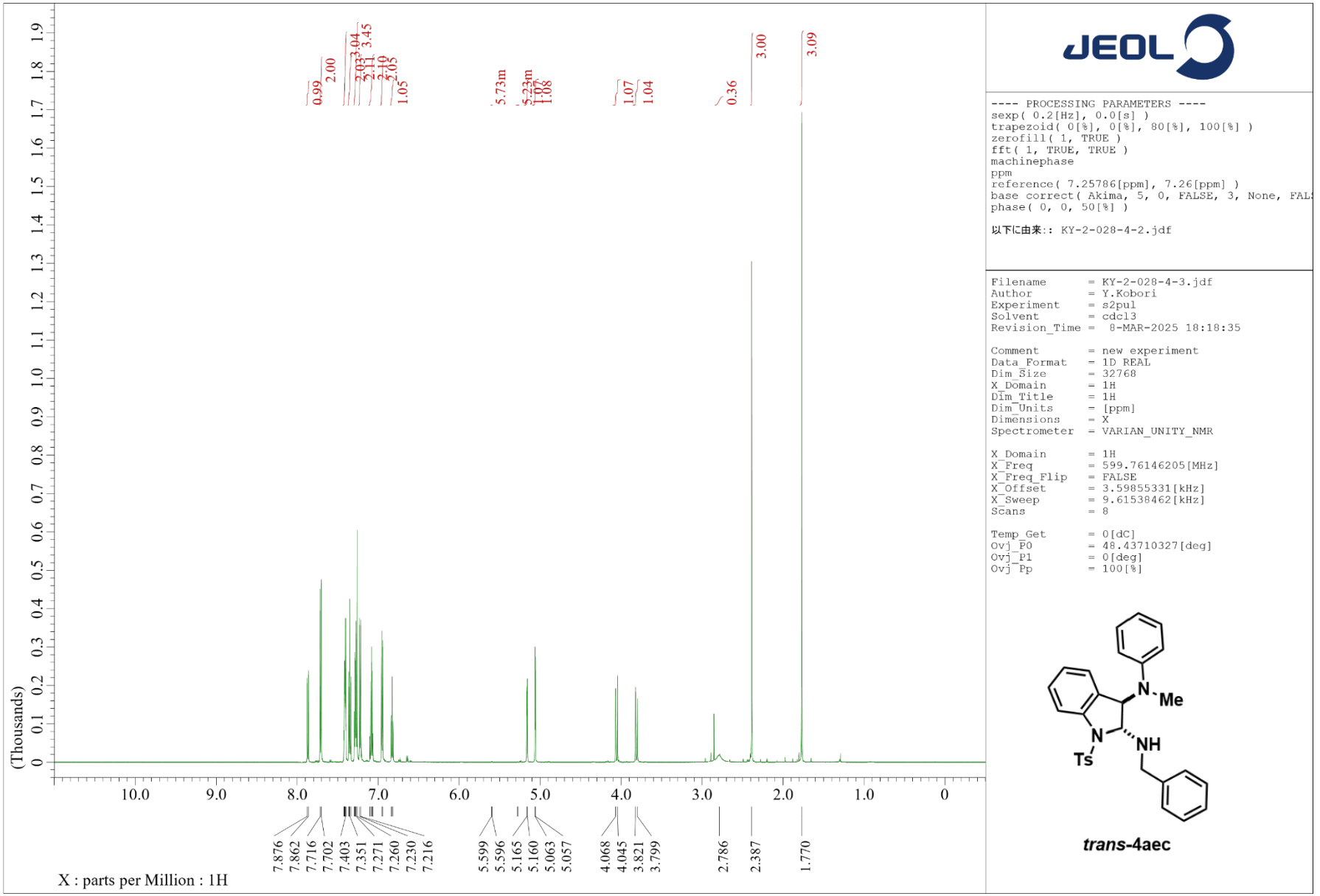
trans-**4adg** **9**

To a mixture of *trans*-**4adg** (217 mg, 0.5 mmol) and MnO_2 (435 mg, 10 equiv., 5.0 mmol) was added DCE (5.0 mL, 0.1 M). The suspension was stirred at reflux in oil bath for 18 h. After the whole was cooled to room temperature, the mixture was filtered through a celite pad. The resulting filtrate was concentrated *in vacuo*. The residue was purified by silica gel column chromatography using AcOEt to give **9** (73.5 mg, 0.27 mmol, 53% yield) as a red solid.

Red solid (73.5 mg, 0.27 mmol, 53% yield; mp 150-152 °C); IR (KBr) ν: 3033, 2966, 2916, 2871, 2852, 1616, 1560, 758, 704 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.41 (t, J = 7.8 Hz, 2H), 7.21 (t, J = 7.2 Hz, 1H), 7.17 (dt, J = 7.8, 1.2 Hz, 1H), 7.03 (d, J = 7.8 Hz, 1H), 6.91 (dd, J = 8.4, 1.2 Hz, 2H), 6.47 (dt, J = 7.2, 1.2 Hz, 1H), 6.32 (d, J = 7.8 Hz, 1H), 3.95 (t, J = 6.0 Hz, 2H), 3.85 (t, J = 6.6 Hz, 2H), 2.02 (q, J = 6.0 Hz, 2H), 1.98 (q, J = 6.6 Hz, 2H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 162.12, 162.12, 160.9, 150.6, 134.3, 129.5, 126.0, 124.7, 120.6, 120.5, 117.7, 117.4, 50.1, 49.0, 26.8, 24.1; HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{18}N_3$ 276.1501; Found 276.1496.

Reference

1) Tokushige, K., Abe, T. *Asian J. Org. Chem.* **2025**, e202500439.
2) (a) Shu, C.; Li, L.; Xiao, X.; Yu, Y.; Ping, Y.; Zhou, J.; Ye, L. *Chem. Commun.* **2014**, 50, 8689-8692; (b) Lin, Q.; Liu, Y.; Song, H.; Wang, Q.; *Adv. Synth. Catal.* **2020**, *362*, 3110-3115; (c) Rivinoja, D.; Gee, Y.; Gardiner, M.; Ryan, J.; Hyland, C.; *ACS Catal.* **2017**, *7*, 1053-1056; (d) Jayaraman, A.; Castro, L.; Fontaine, F.; *Org. Process Res. Dev.* **2018**, *22*, 1489-1499; (e) Tokushige, K.; Kobori, Y.; Asai, S. Abe, T.; *Org. Biiomol. Chem.* **2024**, *22*, 7343-7348.
3) (a) Abe, T.; Suzuki, T.; Anada, M.; Matsunaga, S.; Yamada, K. *Org. Lett.* **2017**, *19*, 4275–4278; (b) Abe, T.; Hirao, S.; Yamashiro, T. *Chem. Commun.* **2020**, *56*, 10183–10186; (c) Abe, T.; Yamashiro, T.; Shimizu, K.; Sawada, D. *Chem. Eur. J.* **2022**, *28*, e202201113; (d) Abe, T.; Yamada, K. *Org. Lett.* **2018**, *20*, 1469–1472.

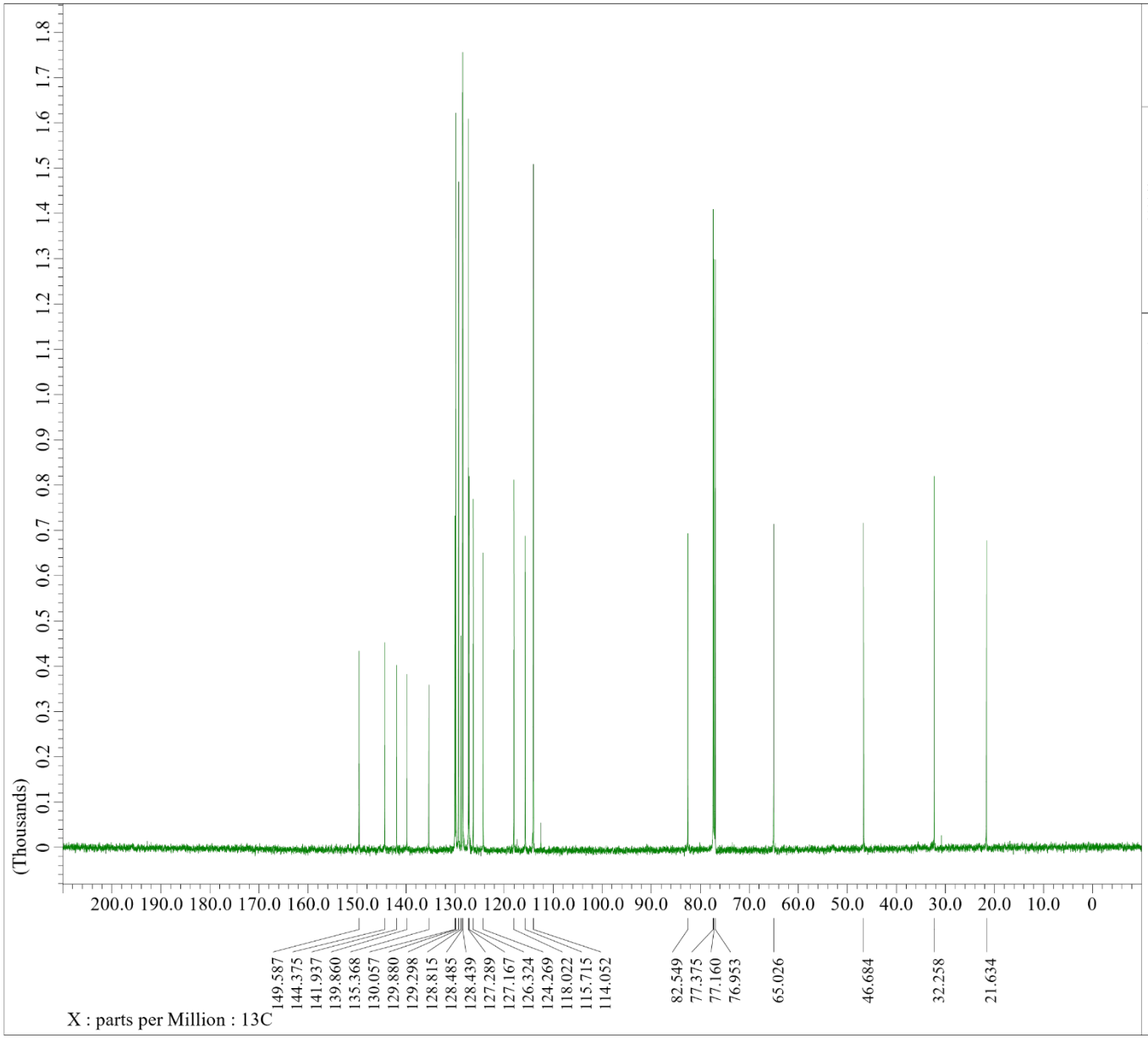


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25786[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-028-4-2.jdf
```

```
Filename       = KY-2-028-4-3.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  =  8-MAR-2025 18:18:35

Comment        = new experiment
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 0[dC]
Ovj_P0         = 48.43710327[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```

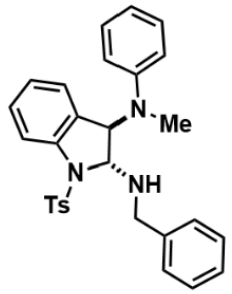

***trans*-4aec**



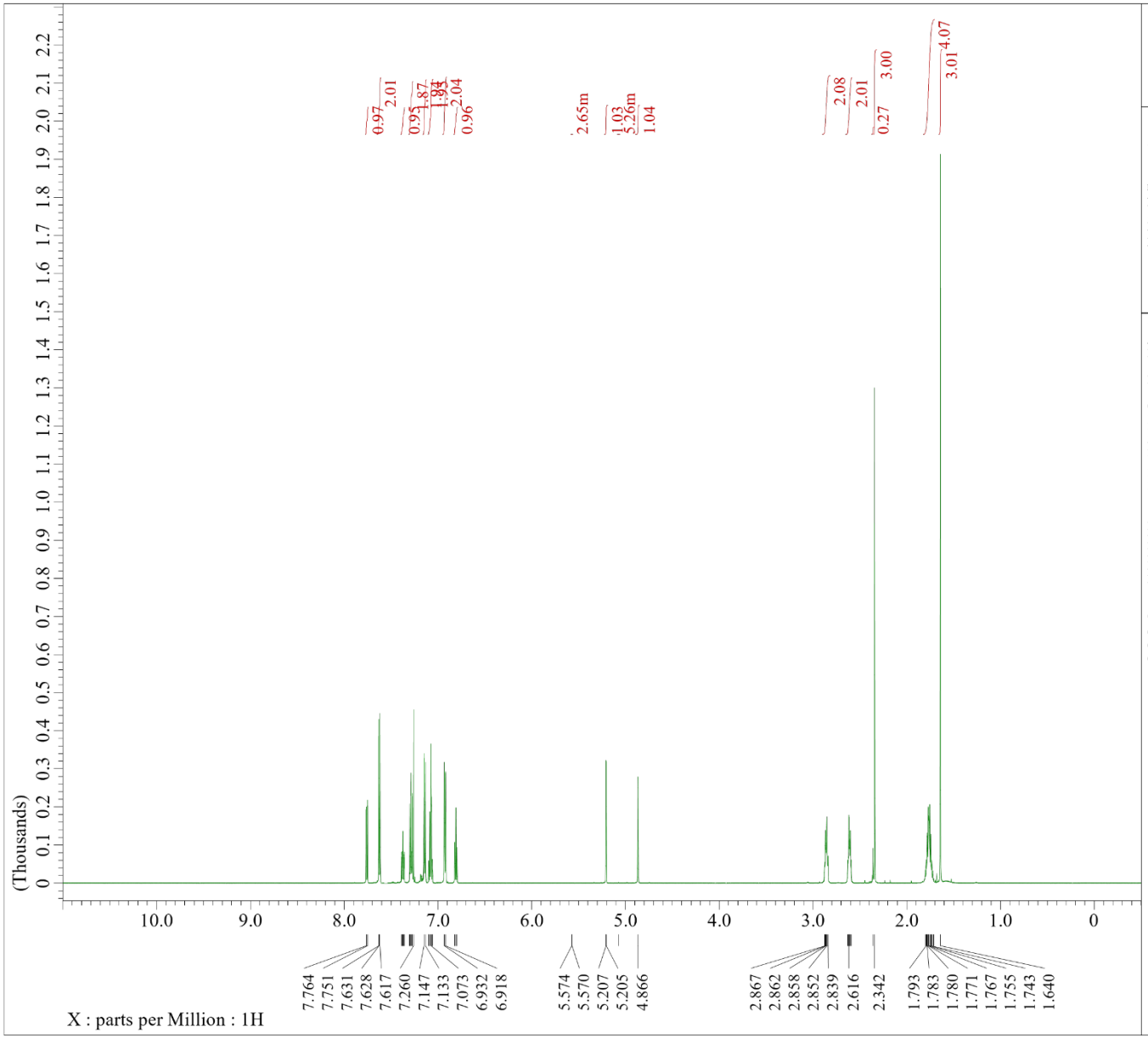
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -8.25, -74, 42.68929[%] )

以下に由来:: KY-2-028-4-carbon-3.jdf
```

```
Filename        = KY-2-028-4-carbon-4.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   = 16-APR-2025 12:01:07

Comment         = 2025/2/7
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
X_Domain        = 13
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 13C
X_Freq          = 150.81013958[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 16.58911607[kHz]
X_Sweep         = 37.87878788[kHz]
Scans           = 256

Temp_Get        = 0[dC]
Ovj_P0          = -84.35593182[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```

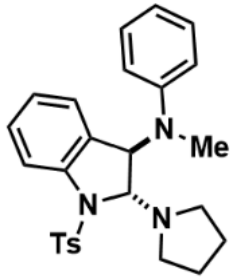


***trans*-4aec**

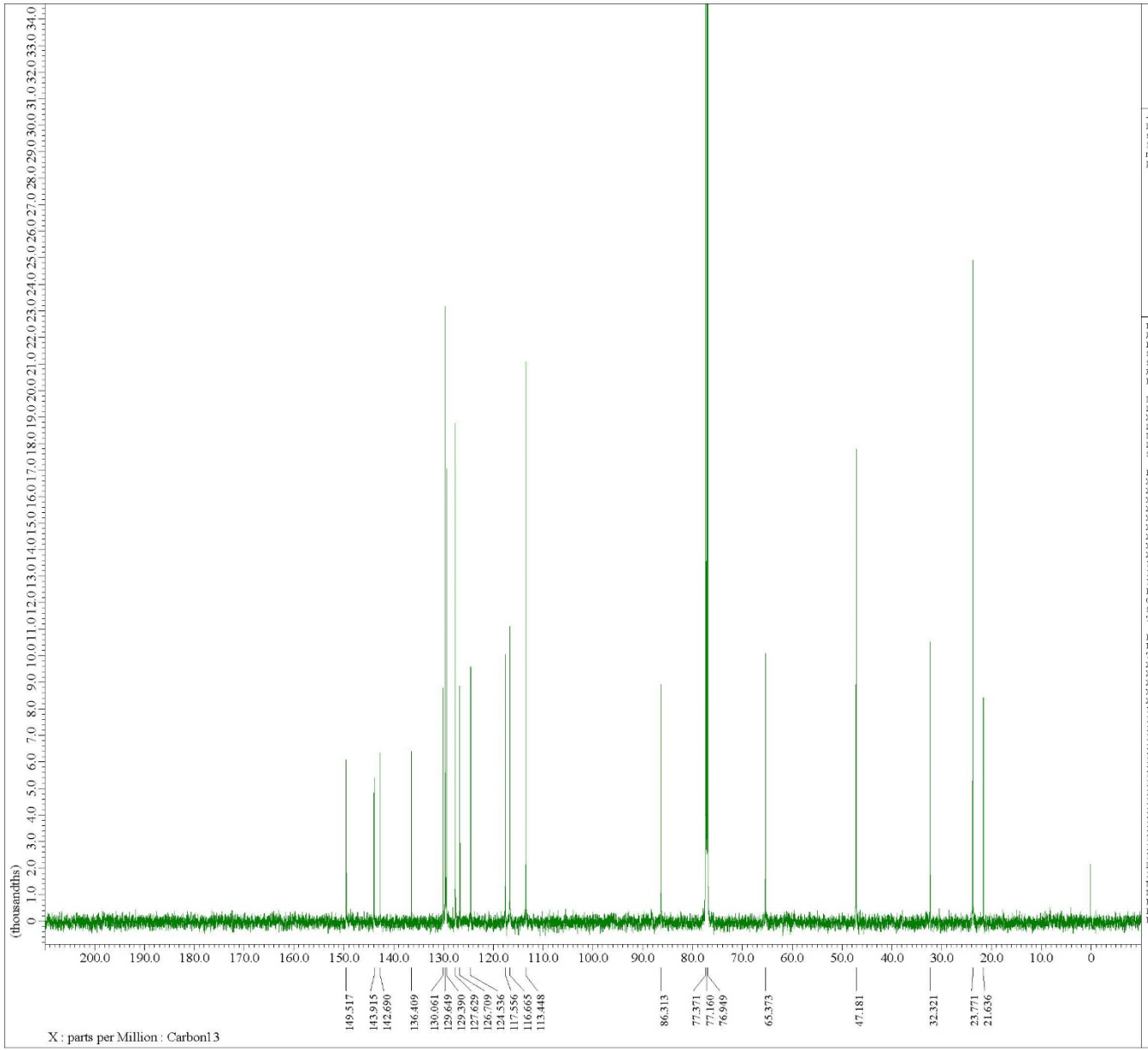



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25786[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-076-1-3.jdf
```

```
Filename        = KY-2-076-1-4.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   =  8-MAR-2025 11:56:59

Comment         = Automated Probe tuning paramet
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 0[dC]
Ovj_P0          = -103.60624497[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```

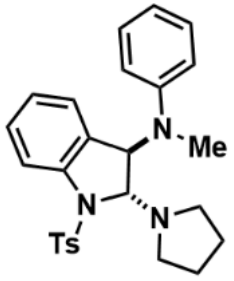


***trans*-4aeg**

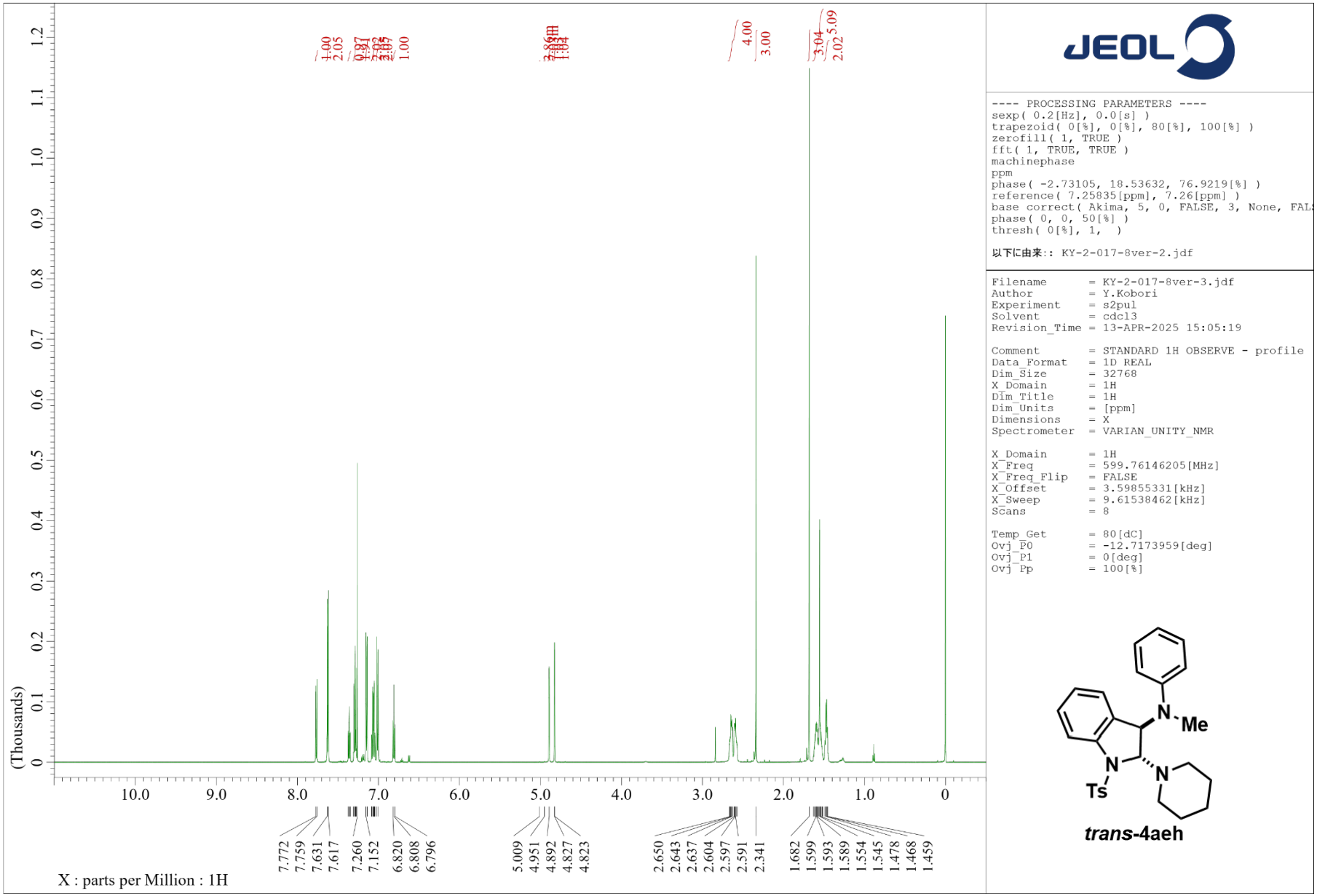


---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm

Filename	= KY-2-151-1(TK)-carbon_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-2-151-1(TK)-carbon
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-APR-2025 02:47:00
Revision_Time	= 26-APR-2025 09:09:56
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15.0[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Set	= 20[dC]
X_90_Width	= 8.1[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 2.7[us]
Irr_Atn_Dec	= 25.803[dB]
Irr_Atn_Dec_Calc	= 25.803[dB]
Irr_Atn_Dec_Default_Calc	= 25.803[dB]
Irr_Atn_Noe	
Irr_Dec_Bandwidth	
Irr_Dec_Bandwidth	
Irr_Dec_Freq	
Irr_Dec_Merit_Fac	
Irr_Decoupling	
Irr_Noe	
Irr_Noise	
Irr_Offset_Defaul	
Irr_Pwidth	
Irr_Pwidth_Defaul	
Irr_Pwidth_Defaul	
Irr_Pwidth_Templ	
Irr_Wurst	
Decimation_Rate	
Initial_Wait	
Noe_Time	
Noe_Time_Flag	
Relaxation_Delay_	
Relaxation_Delay_	
Repetition_Time	



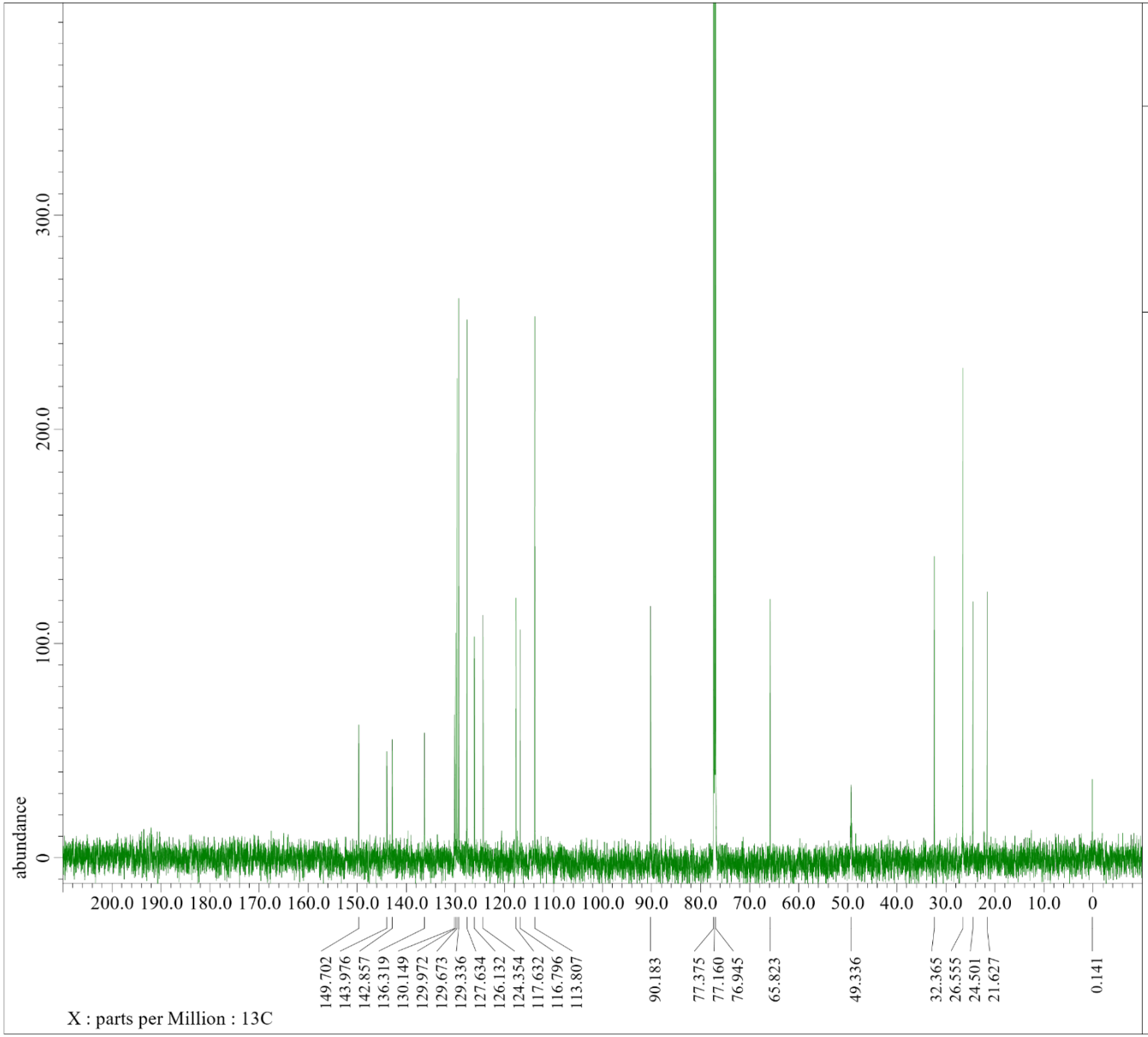
***trans*-4aeg**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -2.73105, 18.53632, 76.9219[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )
thresh( 0[%], 1,  )

以下に由来:: KY-2-017-8ver-2.jdf
```

```
Filename       = KY-2-017-8ver-3.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 13-APR-2025 15:05:19

Comment        = STANDARD 1H OBSERVE - profile
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = -12.7173959[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```

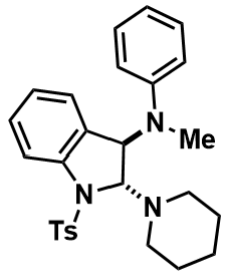

***trans*-4aeh**



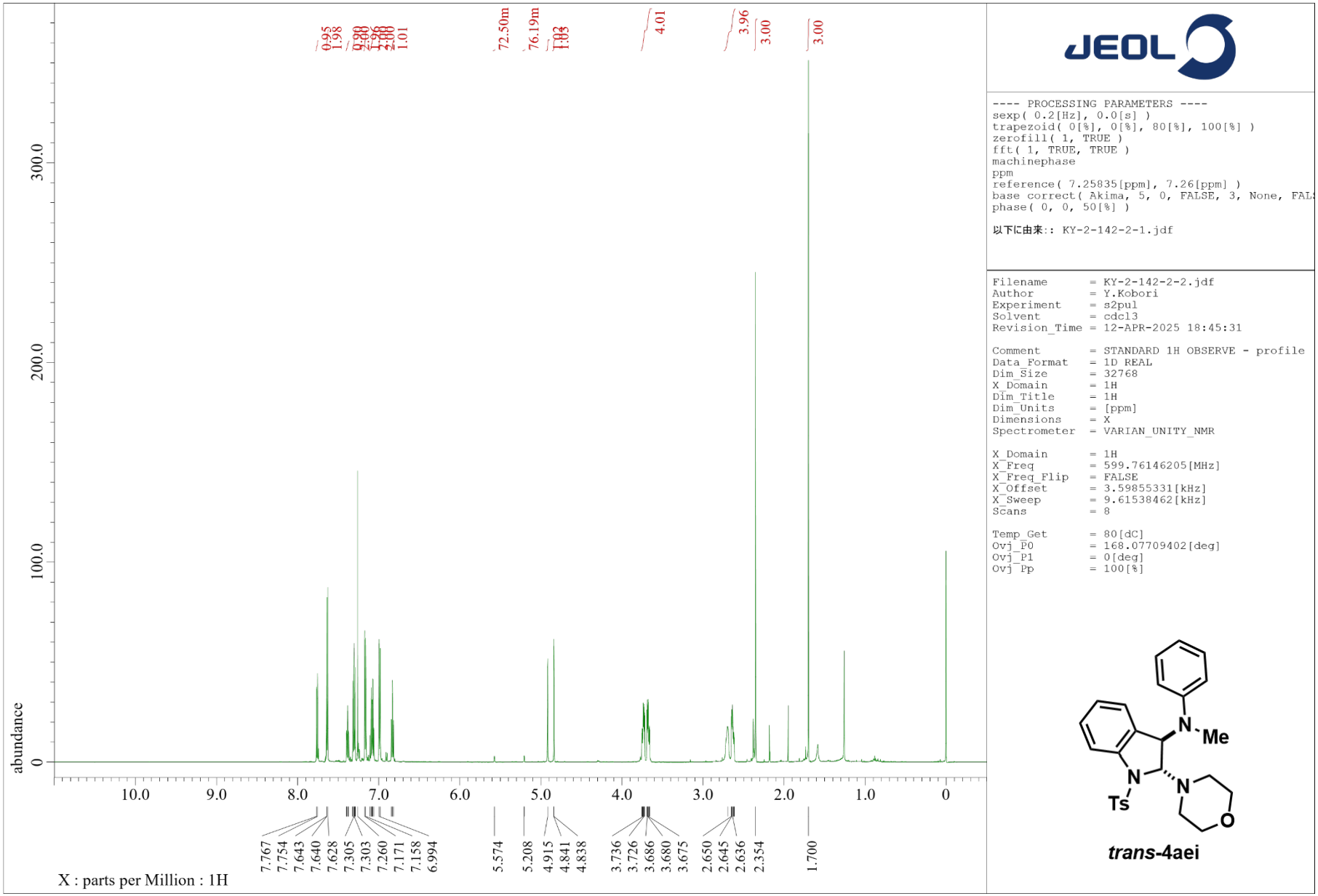
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.00958[ppm], 77.16[ppm] )
phase( 0, 0, 50[%] )
thresh( 1.93132[%], 1.93132[%],  )

以下に由来:: KY-2-017-8ver.2-carbon-2.jdf
```

```
Filename       = KY-2-017-8ver.2-carbon-3.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 21-APR-2025 09:52:33

Comment        = STANDARD 1H OBSERVE - profile
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
X_Domain       = 13
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 13C
X_Freq         = 150.81013958[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 16.58911607[kHz]
X_Sweep        = 37.87878788[kHz]
Scans          = 256

Temp_Get       = 80[dC]
Ovj_P0         = -65.361269[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```



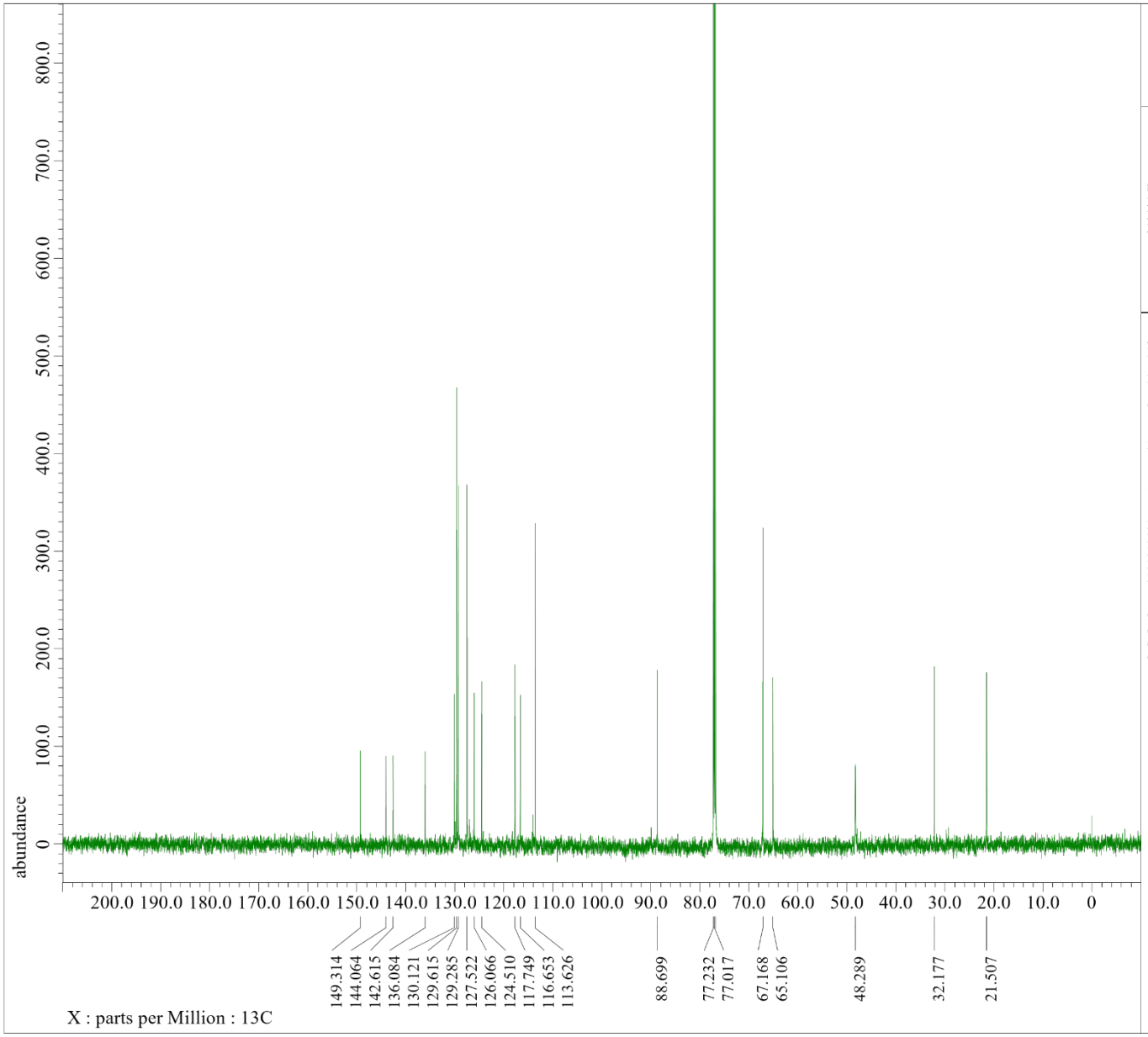
***trans*-4aeh**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-142-2-1.jdf
```

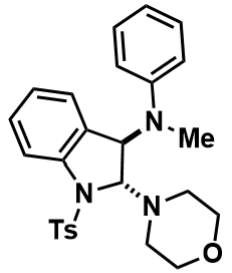
```
Filename       = KY-2-142-2-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 12-APR-2025 18:45:31

Comment        = STANDARD 1H OBSERVE - profile
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = 168.07709402[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```


***trans*-4aei**

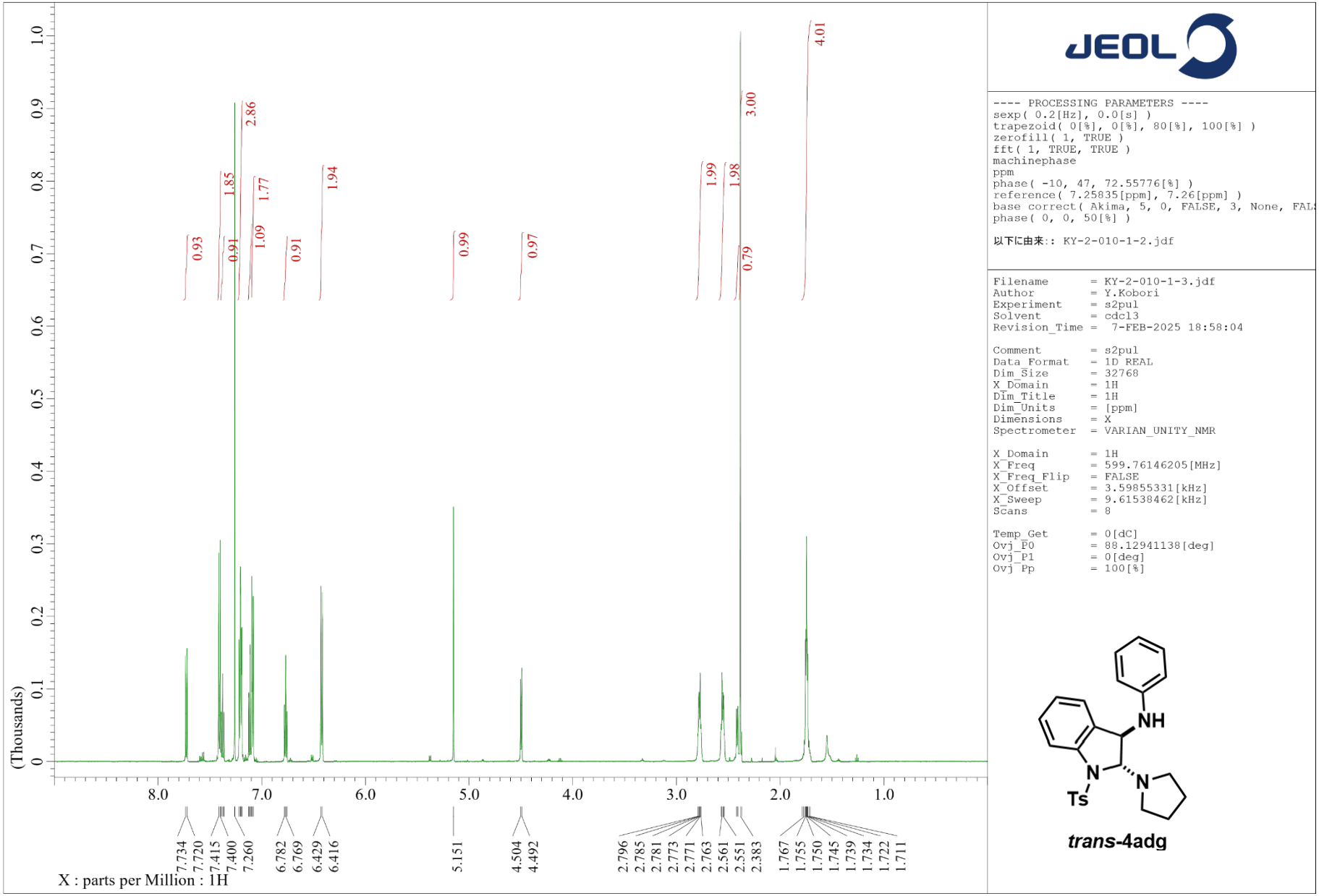



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -0.65589, -133.10984, 63.04819[%] )
phase( 0, 0, 50[%] )

以下に由来:: KY-2-142-2-carbon-2.jdf
```

```
Filename       = KY-2-142-2-carbon-3.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 13-APR-2025 14:03:21

Comment        = STANDARD 1H OBSERVE - profile
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
X_Domain       = 13
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 13C
X_Freq         = 150.81013958[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 16.58911607[kHz]
X_Sweep        = 37.87878788[kHz]
Scans          = 256

Temp_Get       = 80[dC]
Ovj_P0         = 114.57616178[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```



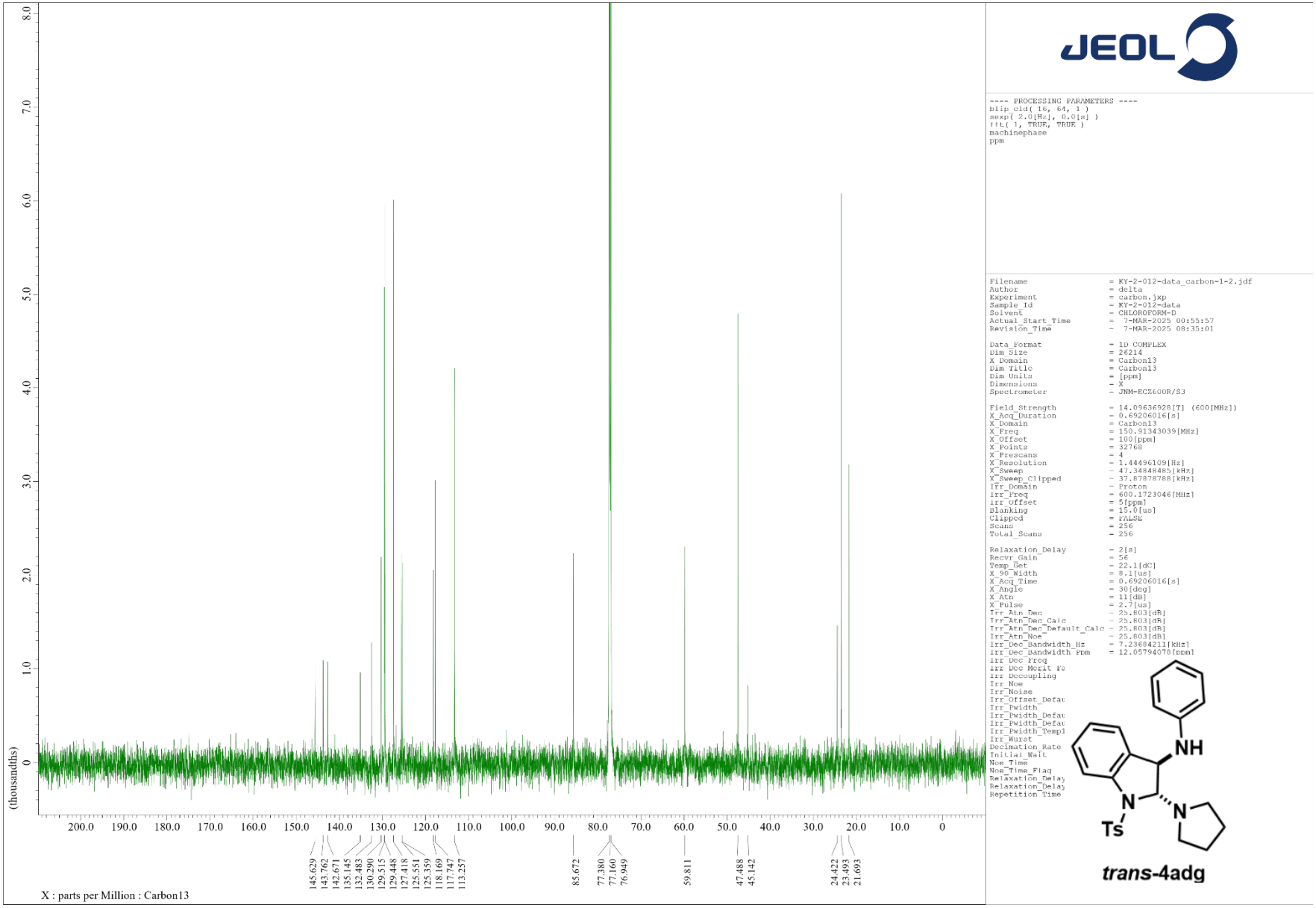
***trans*-4aei**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -10, 47, 72.55776[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-010-1-2.jdf
```

```
Filename        = KY-2-010-1-3.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   =  7-FEB-2025 18:58:04

Comment         = s2pul
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 0[dC]
Ovj_P0          = 88.12941138[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```


***trans*-4adg**



---- PROCESSING PARAMETERS ----
blip cid(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm

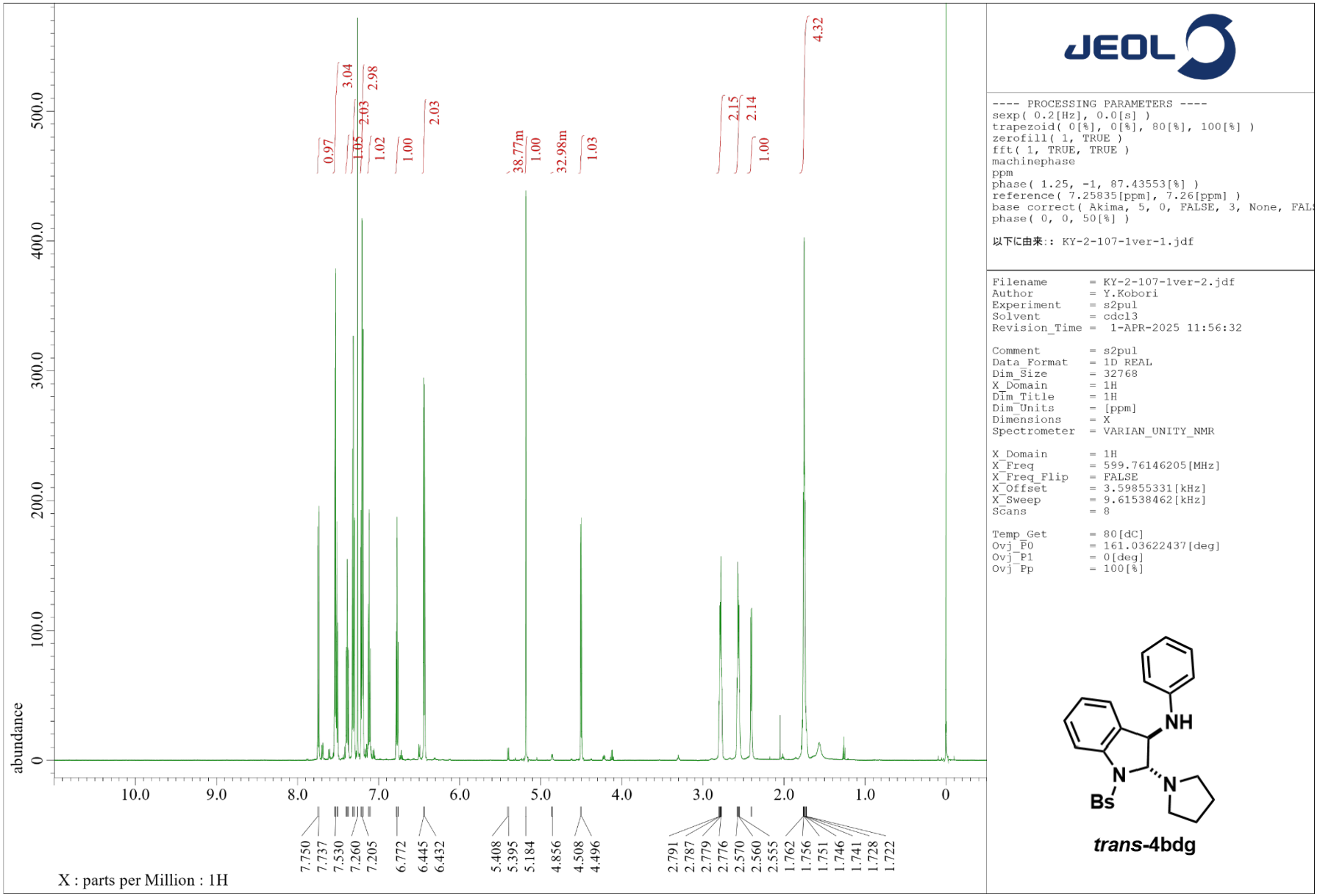
Filename = KY-2-012-data_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = KY-2-012-data
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-MAR-2025 00:55:57
Revision_Time = 7-MAR-2025 08:35:01

Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 15.0[us]
Clipped = FALSE
Scans = 256
Total_Scans = 256

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.1[dC]
X_90_Width = 8.1[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 11[dB]
X_Pulse = 2.7[us]
Irr_Atn_Dec = 25.803[dB]
Irr_Atn_Dec_Calc = 25.803[dB]
Irr_Atn_Dec_Default_Calc = 25.803[dB]
Irr_Atn_Noe = 25.803[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794076[ppm]
Irr_Dec_Freq
Irr_Dec_Merit_Fo
Irr_Decoupling
Irr_Noe
Irr_Noise
Irr_Offset_Defau
Irr_Pwidth
Irr_Pwidth_Defau
Irr_Pwidth_Defau
Irr_Pwidth_Templ
Irr_Wurst
Decimation_Rate
Initial_Wait
Noe_Time
Noe_Time_Flag
Relaxation_Delay
Relaxation_Delay
Repetition_Time

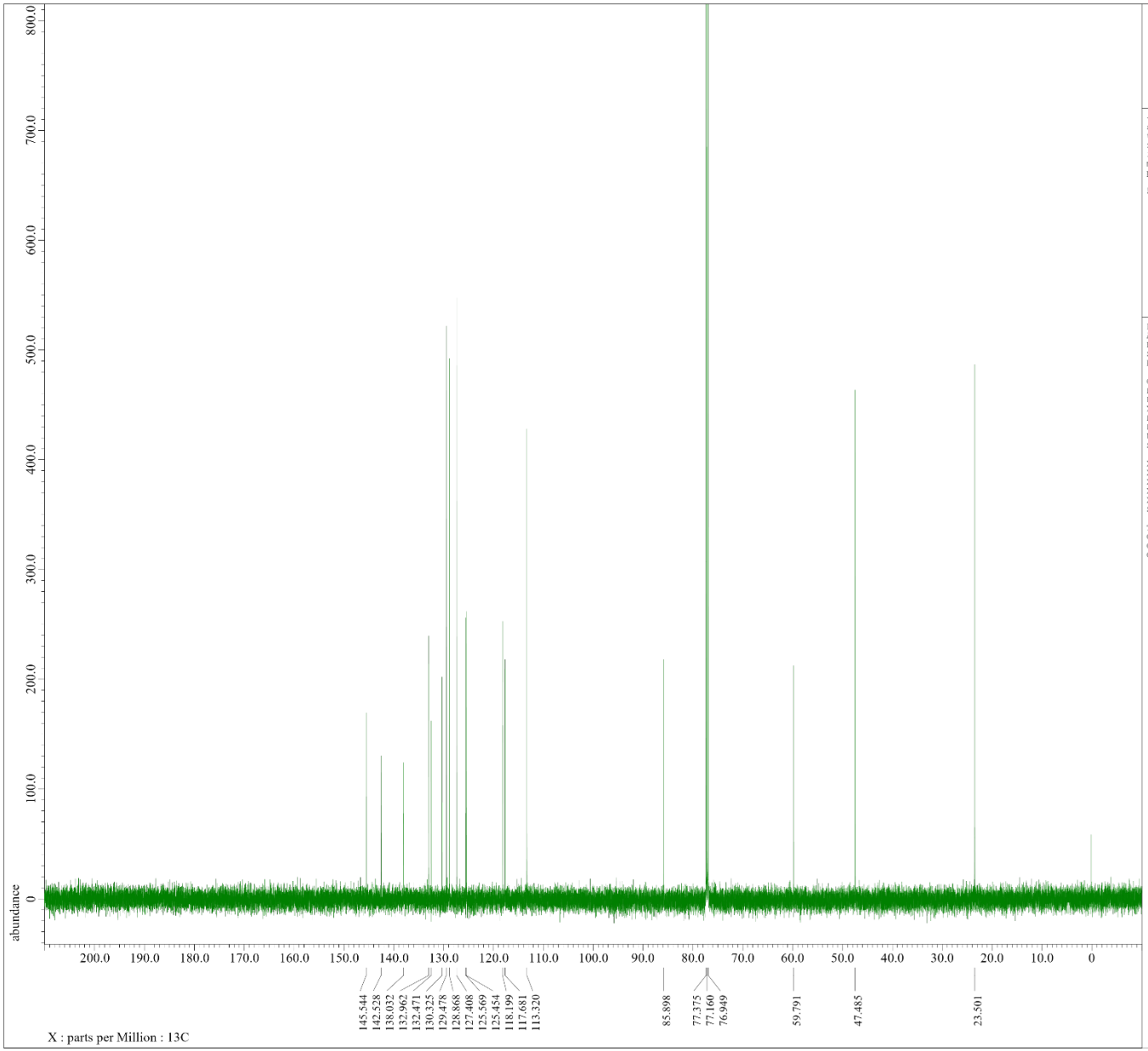
***trans*-4adg**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 1.25, -1, 87.43553[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-107-1ver-1.jdf
```

```
Filename       = KY-2-107-1ver-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  =  1-APR-2025 11:56:32

Comment        = s2pul
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = 161.03622437[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```


***trans*-4bdg**



---- PROCESSING PARAMETERS ----
sexp(0.1[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm

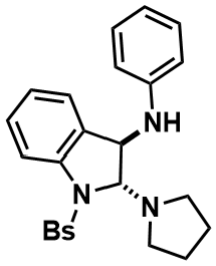
以下に由来:: KY-2-107-1ver.2-carbon-1.jdf

Filename = KY-2-107-1ver.2-carbon-2.jdf
Author = 德里魔祐
Experiment = s2pul
Solvent = cdcl3
Revision_Time = 24-APR-2025 11:42:13

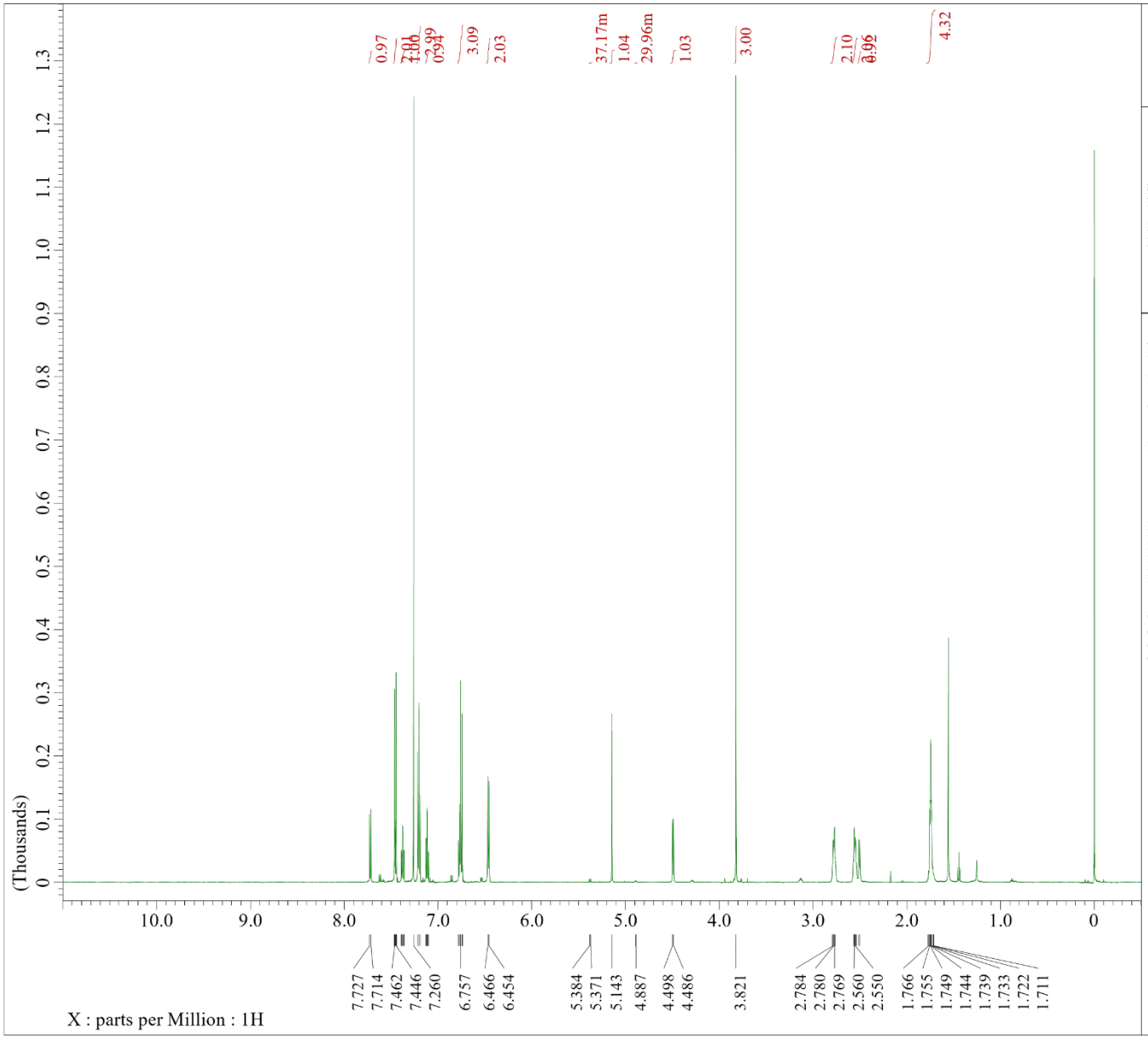
Comment = s2pul
Data Format = 1D COMPLEX
Dim_Size = 65536
X_Domain = 13
Dim Title = 13C
Dim Units = [ppm]
Dimensions = X
Spectrometer = VARIAN_UNITY_NMR

X_Domain = 13C
X_Freq = 150.81013958[MHz]
X_Freq_Flip = FALSE
X_Offset = 16.58911607[kHz]
X_Sweep = 37.87878788[kHz]
Scans = 256

Temp_Get = 60[dC]
Ovj_P0 = 112.24594489[deg]
Ovj_P1 = 0[deg]
Ovj_Pp = 100[%]



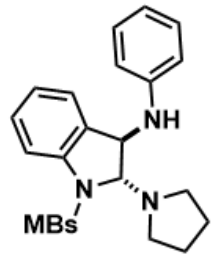
***trans*-4bdg**



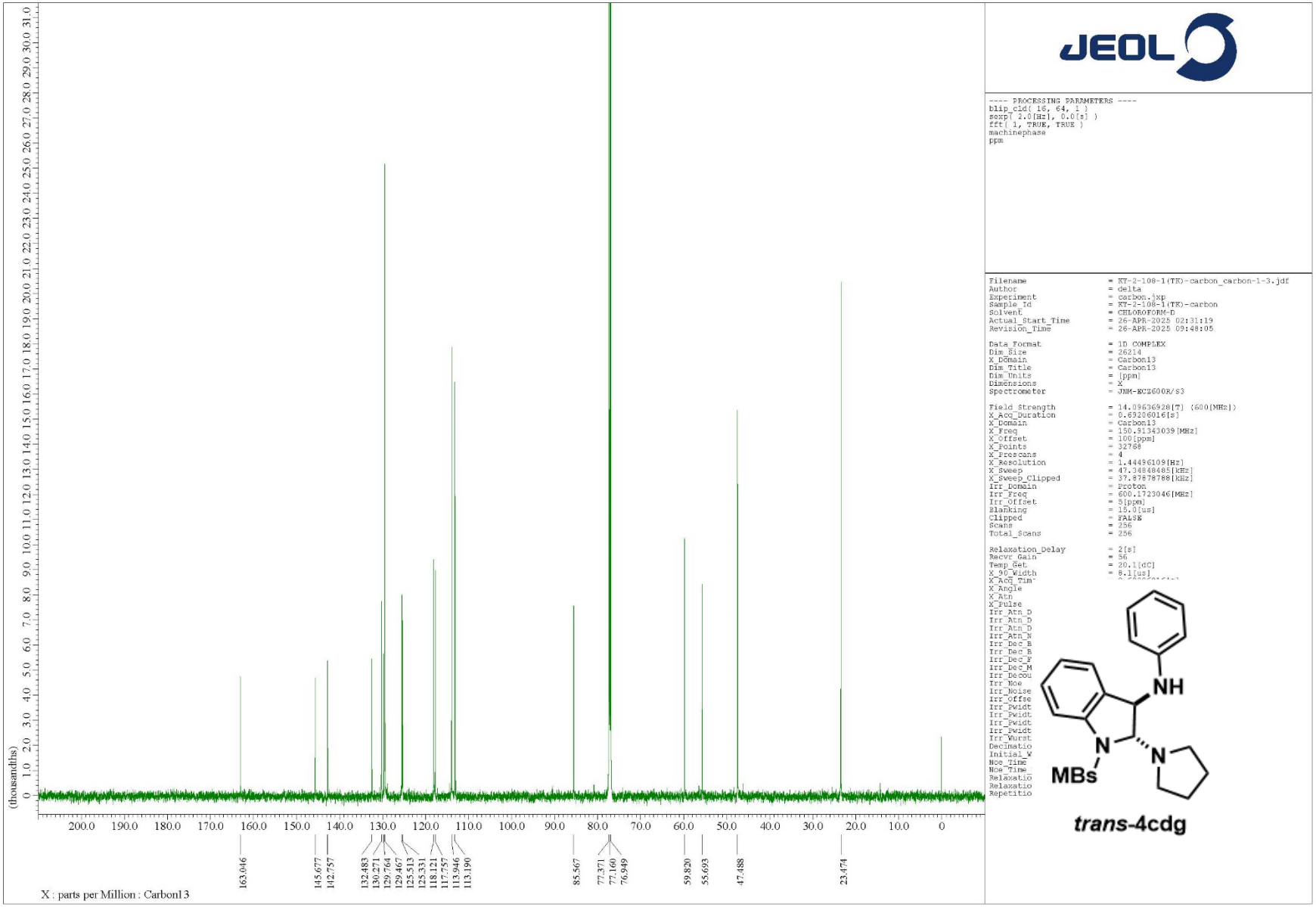
JEOL

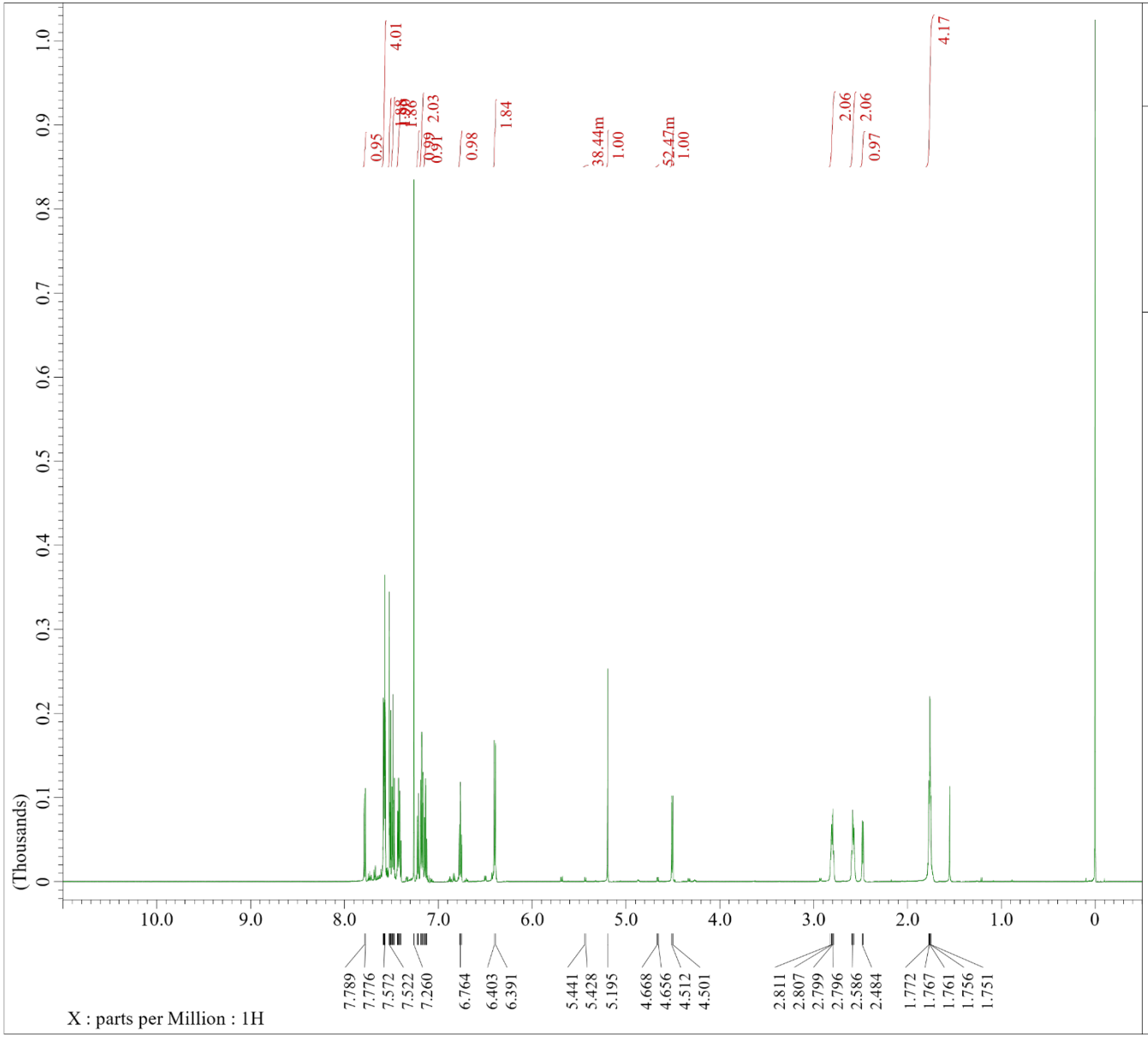
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-108-1ver-5.jdf
```

```
Filename        = KY-2-108-1ver-6.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   =  4-APR-2025 17:17:38

Comment         = s2pul
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 80[dC]
Ovj_P0          = 168.4550596[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```



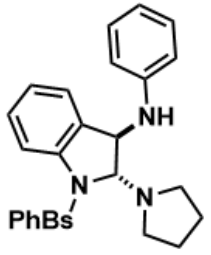
***trans*-4cdg**


(thousandths)
X : parts per Million : Carbon13
163.046
145.677
142.757
132.483
130.271
129.764
129.467
125.513
125.331
118.121
117.757
113.946
113.190
85.567
77.371
77.160
76.949
59.820
55.693
47.488
23.474
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = KY-2-108-1(TK)-carbon_carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = KY-2-108-1(TK)-carbon
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-APR-2025 02:31:19
Revision_Time = 26-APR-2025 09:48:05
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 15.0[us]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.1[dC]
X_90_Width = 8.1[us]
X_Acq_Tim
X_Angle
X_Atn
X_Pulse
Irr_Atn_D
Irr_Atn_D
Irr_Atn_D
Irr_Atn_N
Irr_Dec_B
Irr_Dec_B
Irr_Dec_F
Irr_Dec_M
Irr_DecOu
Irr_Noe
Irr_Noise
Irr_Offse
Irr_Pwidt
Irr_Pwidt
Irr_Pwidt
Irr_Pwidt
Irr_Wurst
DecImatio
Initial_W
Noe_Time
Noe_Time
Relaxatio
Relaxatio
Repetitio
NH
N
N
MBs
trans-4cdg

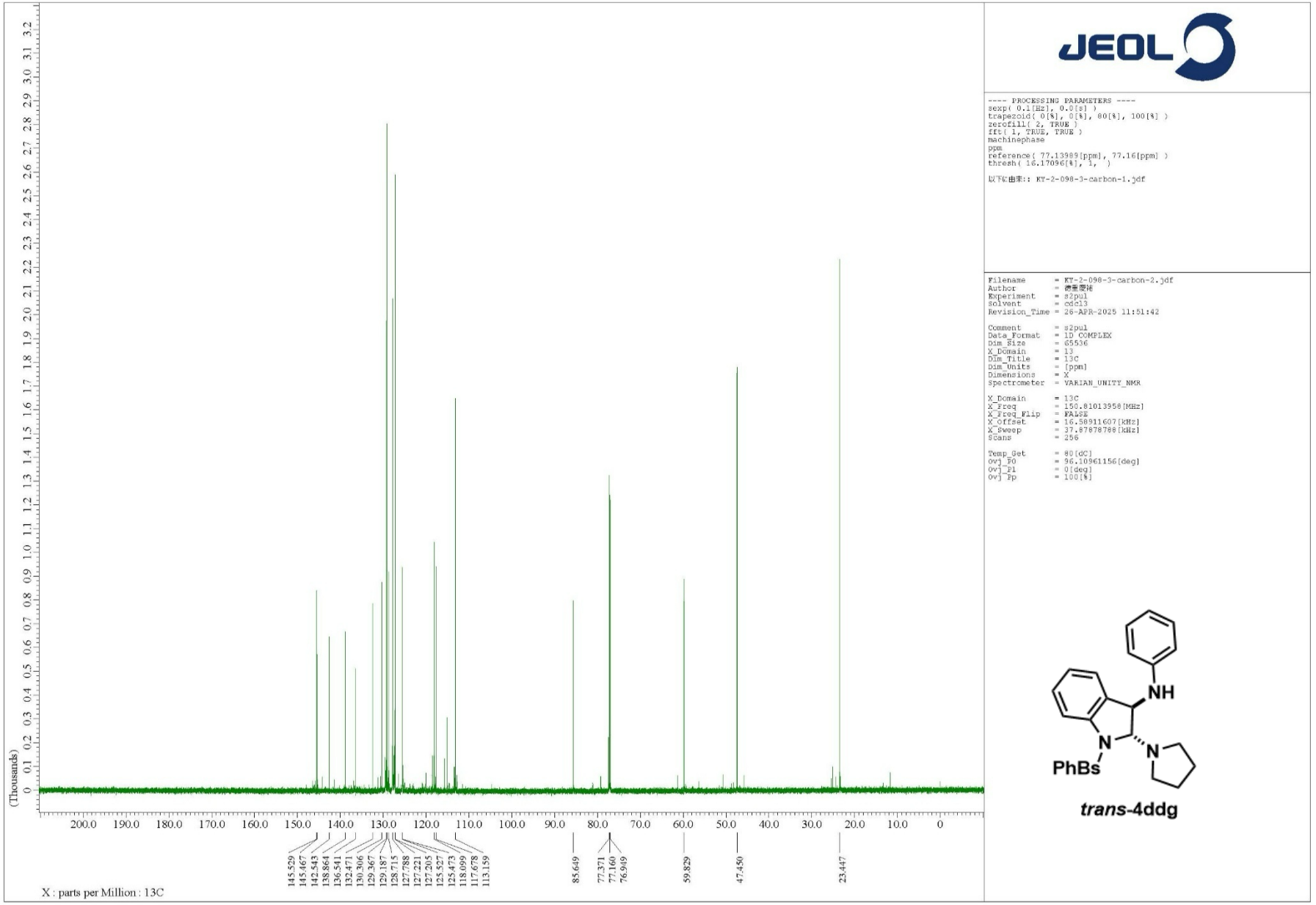



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -3, -3, 87.42637[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-098-7-1.jdf
```

```
Filename       = KY-2-098-7-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  =  9-APR-2025 14:05:21

Comment        = ST-462-2
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = 157.40833104[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```



***trans*-4ddg**



---- PROCESSING PARAMETERS ----
sexp(0.1[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(77.13989[ppm], 77.16[ppm])
thresh(16.17096[%], 1,)

以下の由来:: KY-2-098-3-carbon-1.jdf

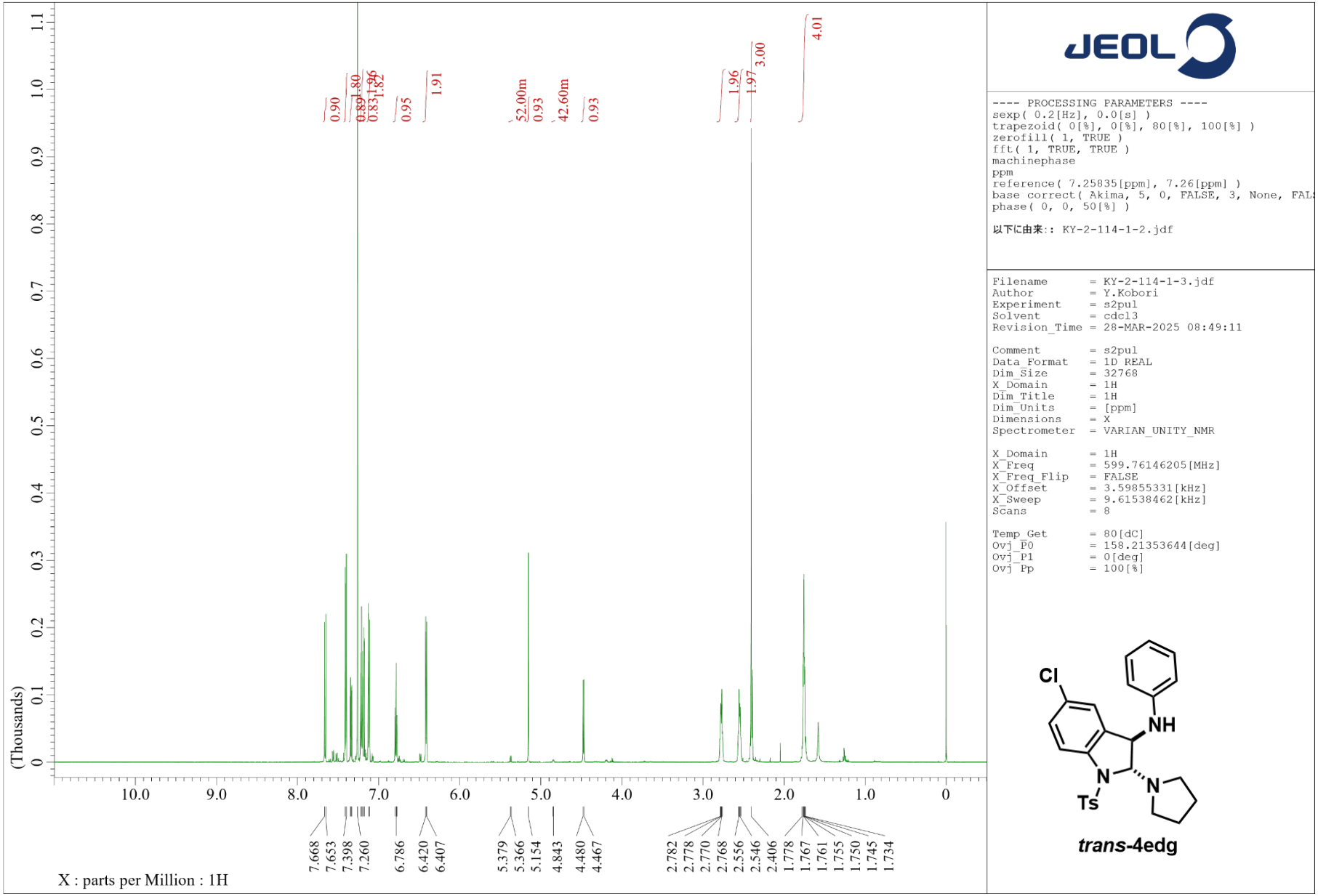
Filename = KY-2-098-3-carbon-2.jdf
Author =
Experiment = s2pul
solvent = cdcl3
Revision_Time = 26-APR-2025 11:51:42

Comment = s2pul
Data_Format = 1D COMPLEX
Dim_Size = 65536
X_Domain = 13
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Spectrometer = VARIAN_UNITY_NMR

X_Domain = 13C
X_Freq = 150.81013958[MHz]
X_Freq_Flip = FALSE
X_Offset = 16.58911607[kHz]
X_Sweep = 37.87878788[kHz]
Scans = 256

Temp_Get = 80[dC]
Ovj_P0 = 96.10961156[deg]
Ovj_P1 = 0[deg]
Ovj_Pp = 100[%]

***trans*-4ddg**

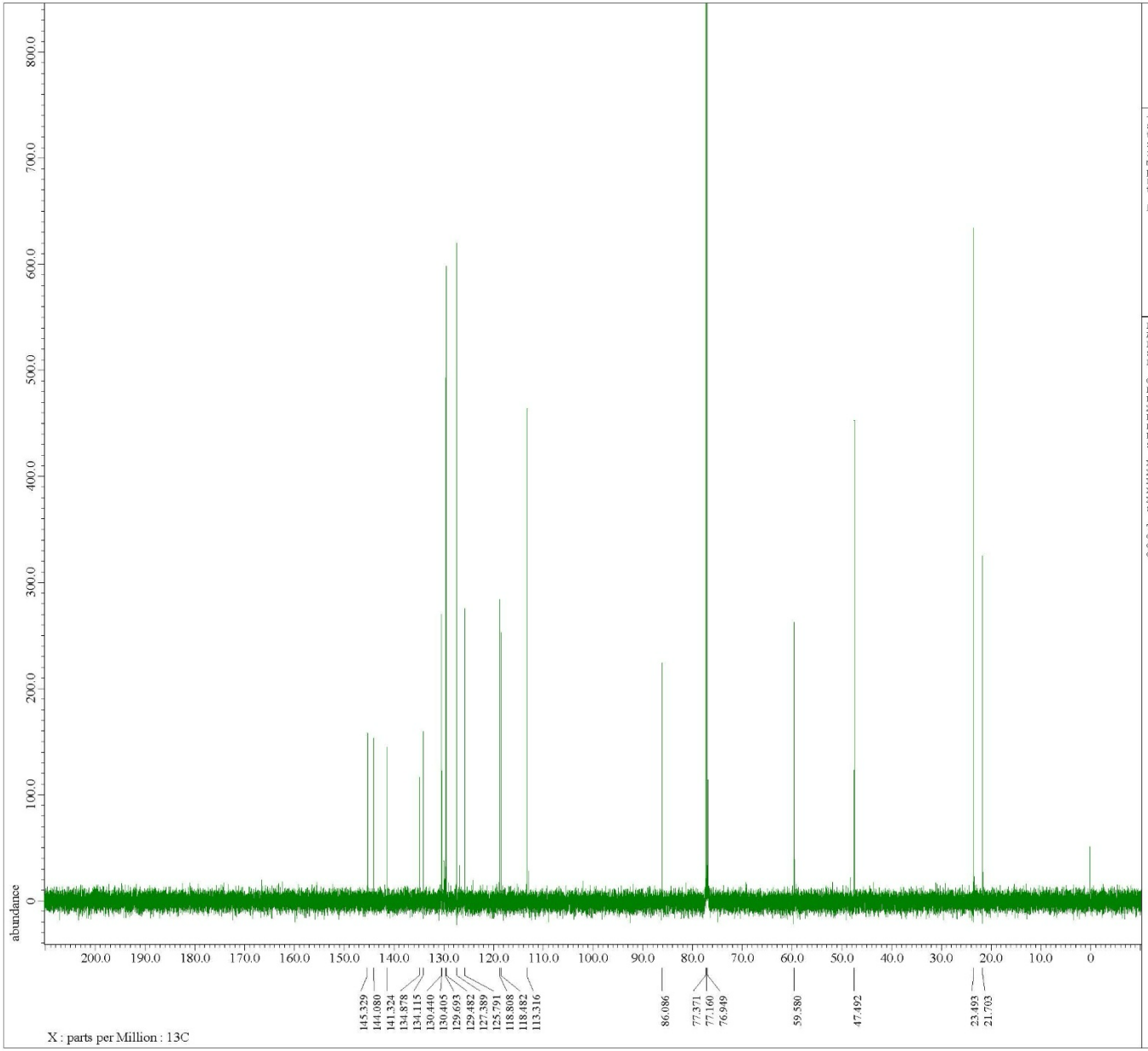


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-114-1-2.jdf
```

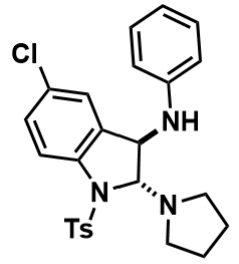
```
Filename       = KY-2-114-1-3.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 28-MAR-2025 08:49:11

Comment        = s2pul
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = 158.21353644[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```


***trans*-4edg**

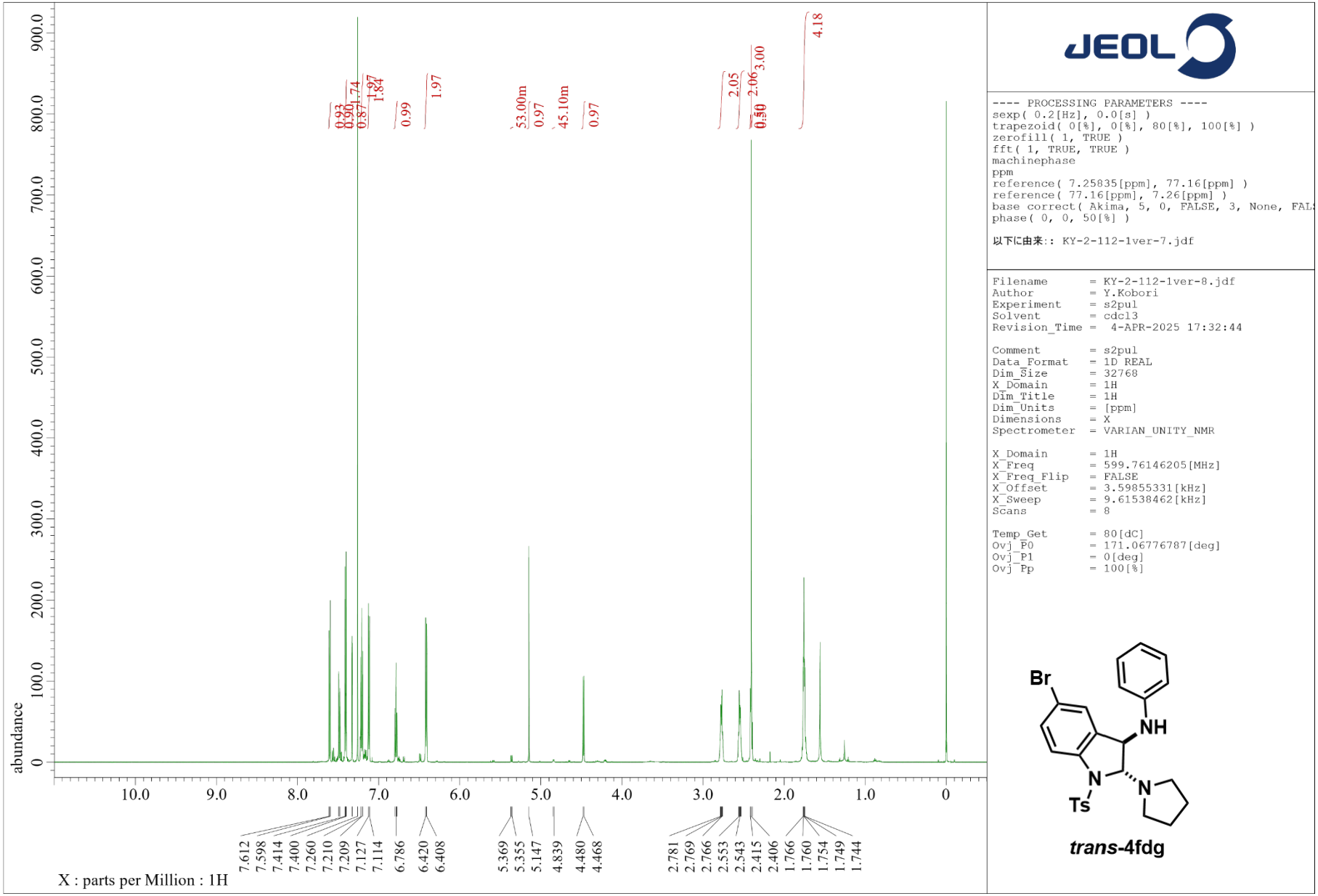



```
---- PROCESSING PARAMETERS ----
sexp( 0.1[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.01725[ppm], 77.16[ppm] )
thresh( 5.87632[%], 2.18798[%], )

以下に由来:: XY-2-114-1-carbon-1.jdf
```

```
Filename        = XY-2-114-1-carbon-2.jdf
Author          = 德重晨祐
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   = 26-APR-2025 11:54:02

Comment         = STANDARD PHOSPHORUS PARAMETERS
Data_Format     = 1D COMPLEX
Dim_Size        = 65536
X_Domain        = 13
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 13C
X_Freq          = 150.81013958[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 16.58911607[kHz]
X_Sweep         = 37.87878788[kHz]
SCans           = 256

Temp_Get        = 80[dC]
Ovj_P0          = 96.10871263[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```



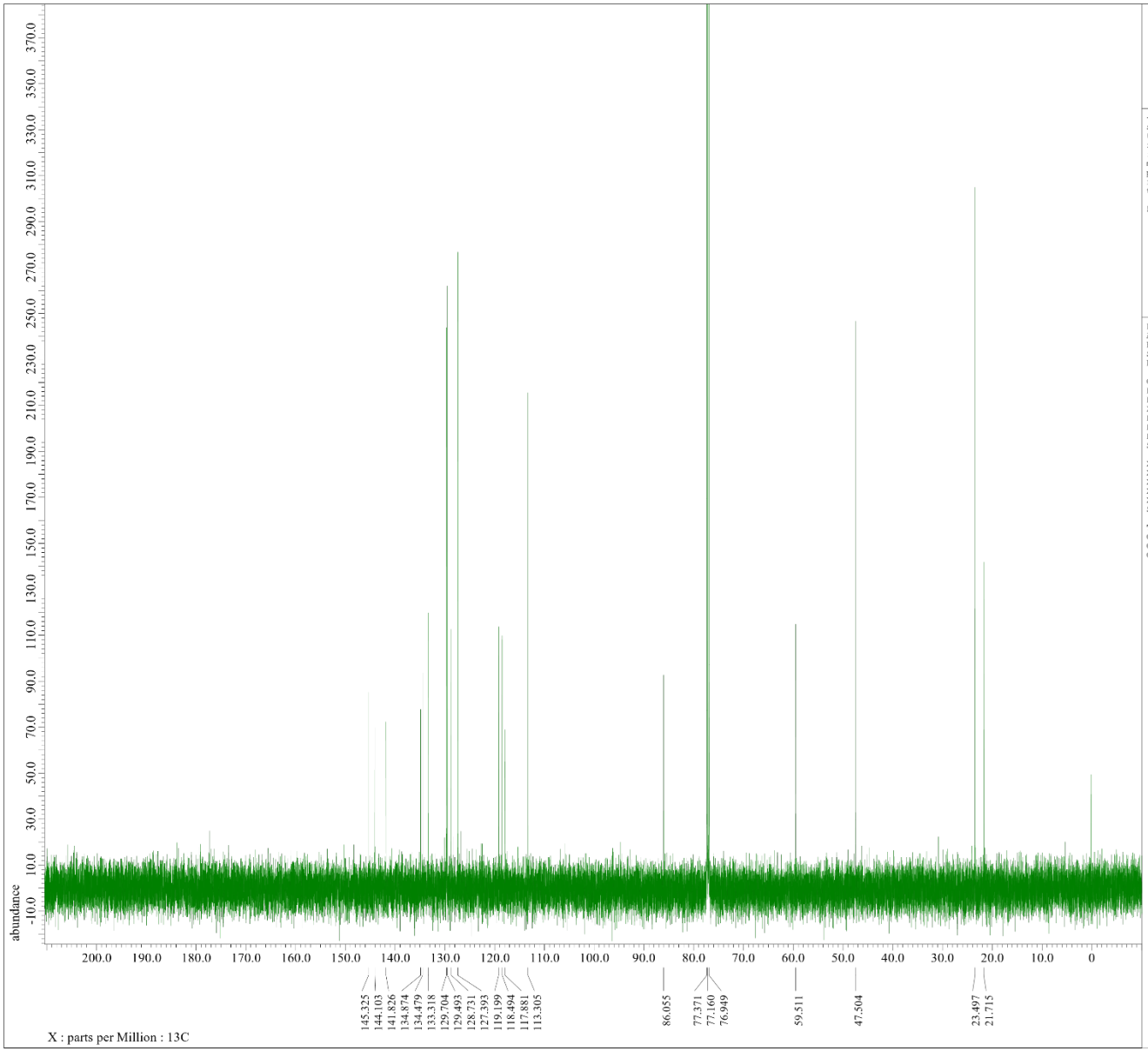
***trans*-4edg**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25835[ppm], 77.16[ppm] )
reference( 77.16[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-112-1ver-7.jdf
```

```
Filename       = KY-2-112-1ver-8.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  =  4-APR-2025 17:32:44

Comment        = s2pul
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = 171.06776787[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```


***trans*-4fdg**



---- PROCESSING PARAMETERS ----
sexp(0.1[Hz], 0.0[sj) trapezoid(0[%], 0[%], 80[%], 100[%]) zerofill(2, TRUE) fft(1, TRUE, TRUE) machinephase ppm reference(77.00958[ppm], 77.16[ppm]) thresh(3.81513[%], 3.2081[%],)

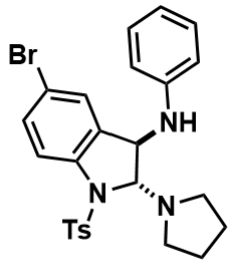
以下に由来:: KY-2-112-1ver.3-carbon-1.jdf

Filename = KY-2-112-1ver.3-carbon-2.jdf
Author = 徳重慶祐
Experiment = s2pul
Solvent = cdcl3
Revision_Time = 24-APR-2025 11:46:07

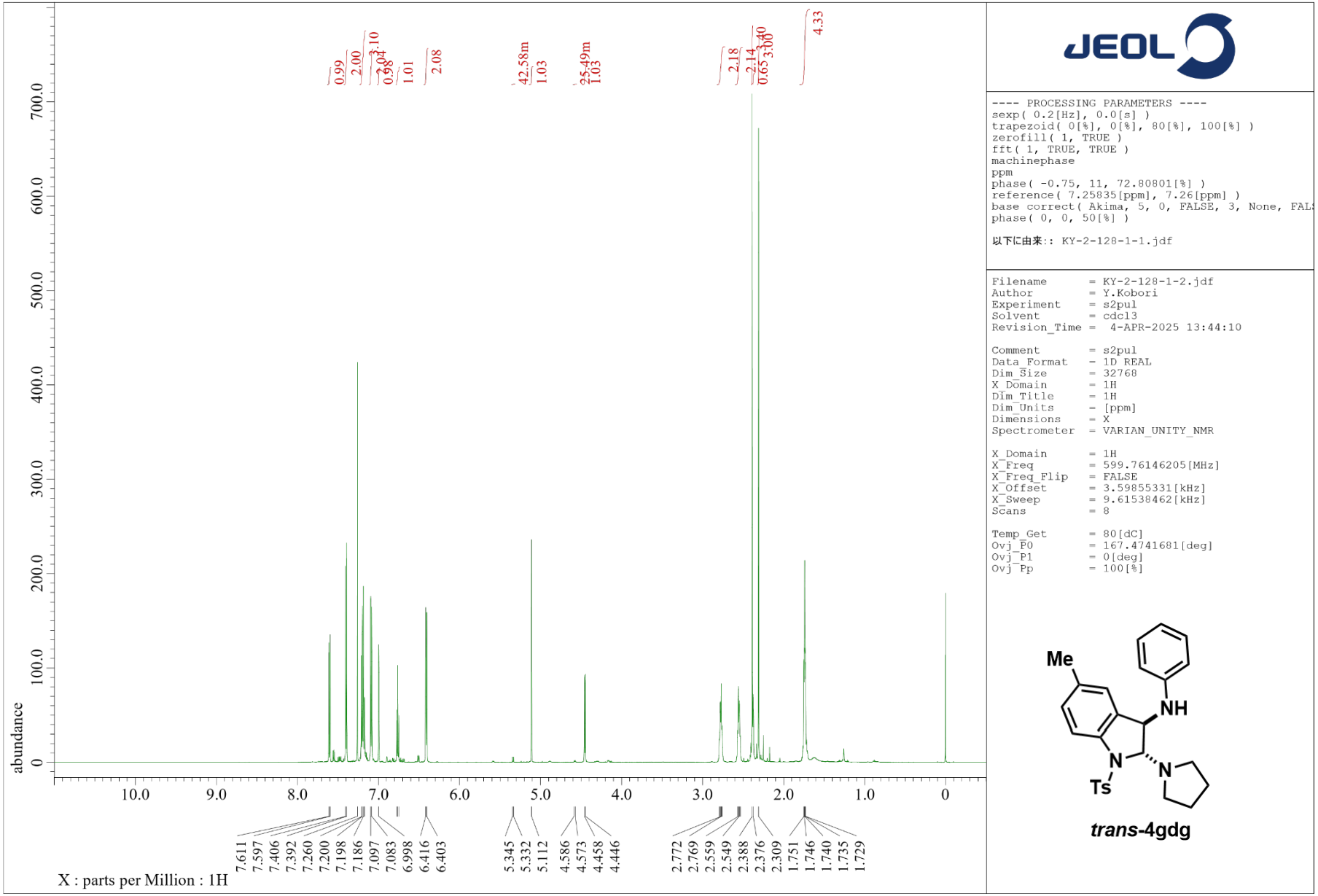
Comment = s2pul
Data_Format = 1D COMPLEX
Dim_Size = 65536
X_Domain = 13
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Spectrometer = VARIAN_UNITY_NMR

X_Domain = 13C
X_Freq = 150.81013950[MHz]
X_Freq_Flip = FALSE
X_Offset = 16.58911607[kHz]
X_Sweep = 37.87878788[kHz]
SCans = 256

Temp_Get = 80[dC]
Ovj_Fn = 96.402648931deqj
Ovj_P1 = 0[deq]
Ovj_Pp = 100[%]



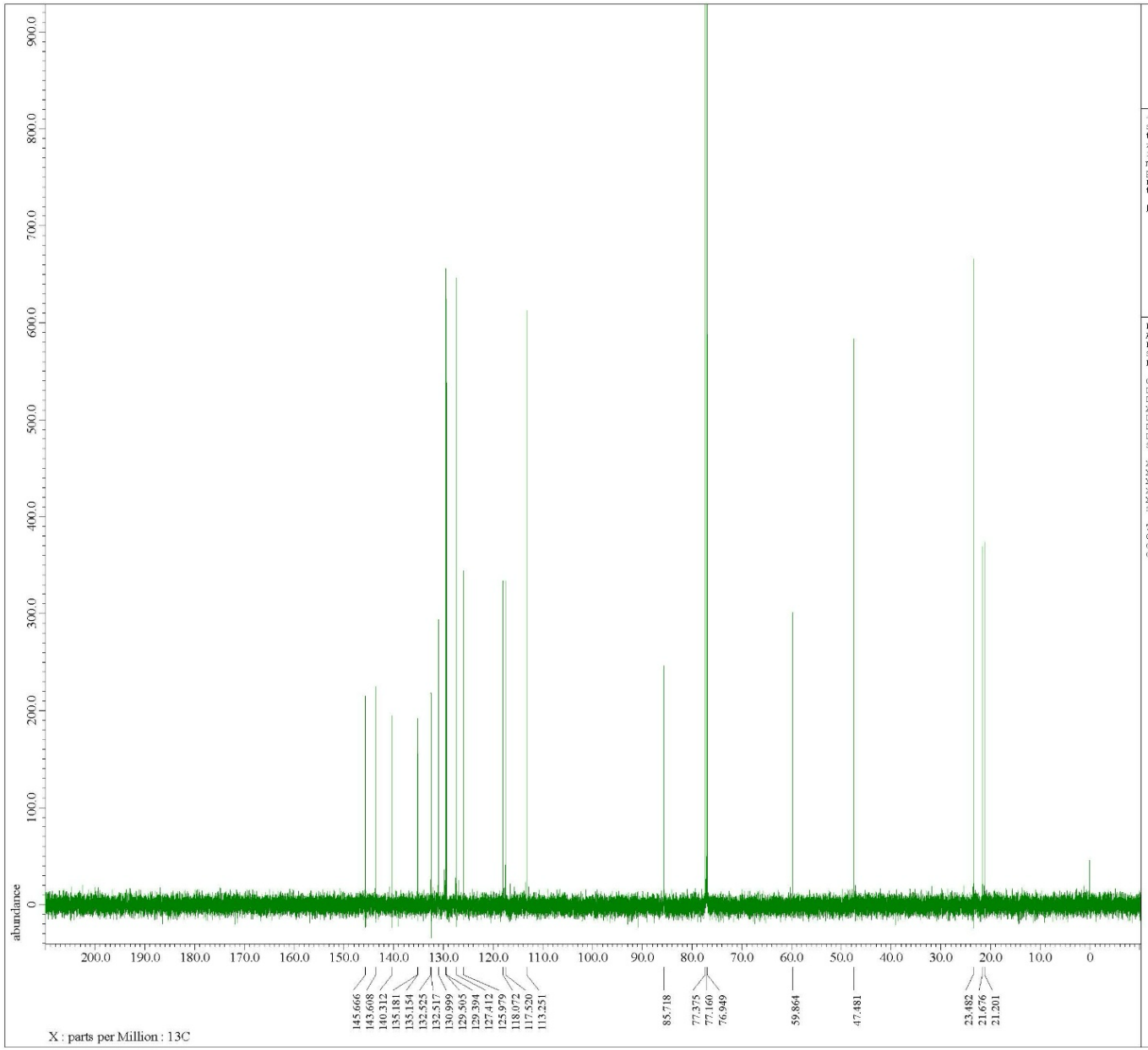
***trans*-4fdg**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -0.75, 11, 72.80801[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-128-1-1.jdf
```

```
Filename        = KY-2-128-1-2.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   =  4-APR-2025 13:44:10

Comment         = s2pul
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 80[dC]
Ovj_P0          = 167.4741681[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```


***trans*-4gdg**



---- PROCESSING PARAMETERS ----
exp(0.1[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(77.02491[ppm], 77.16[ppm])
thresh(3.78402[%], 3.02722[%], 21.23435[abn])

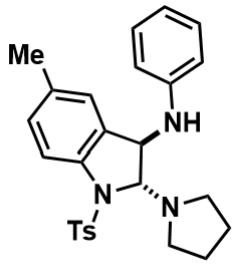
以下に由来:: KY-2-128-1-carbon-1.jdf

Filename = KY-2-128-1-carbon-2.jdf
Author = 清水愛祐
Experiment = s2pul
Solvent = cdcl3
Revision_Time = 26-APR-2025 11:55:30

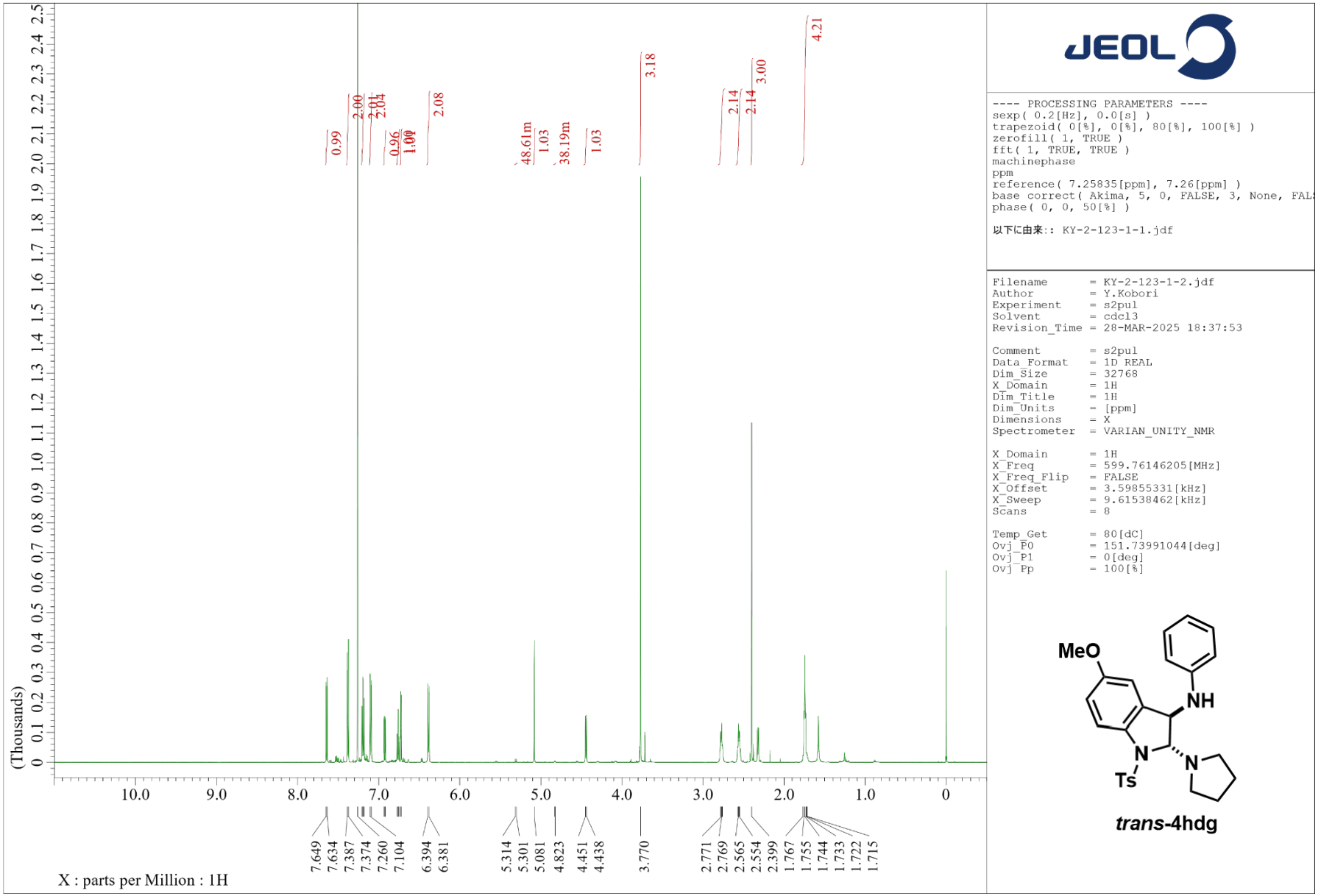
Comment = s2pul
Data_Format = 1D COMPLEX
Dim_Size = 65536
X_Domain = 13
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Spectrometer = VARIAN_UNITY_NMR

X_Domain = 13C
X_Freq = 150.81013958[MHz]
X_Freq_Flip = FALSE
X_Offset = 16.58911607[kHz]
X_Sweep = 37.87878788[kHz]
Scans = 256

Temp_Set = 80[dC]
Cvj_P0 = 101.80127989[deg]
Cvj_P1 = 0[deg]
Cvj_Pp = 100[%]



***trans*-4gdg**

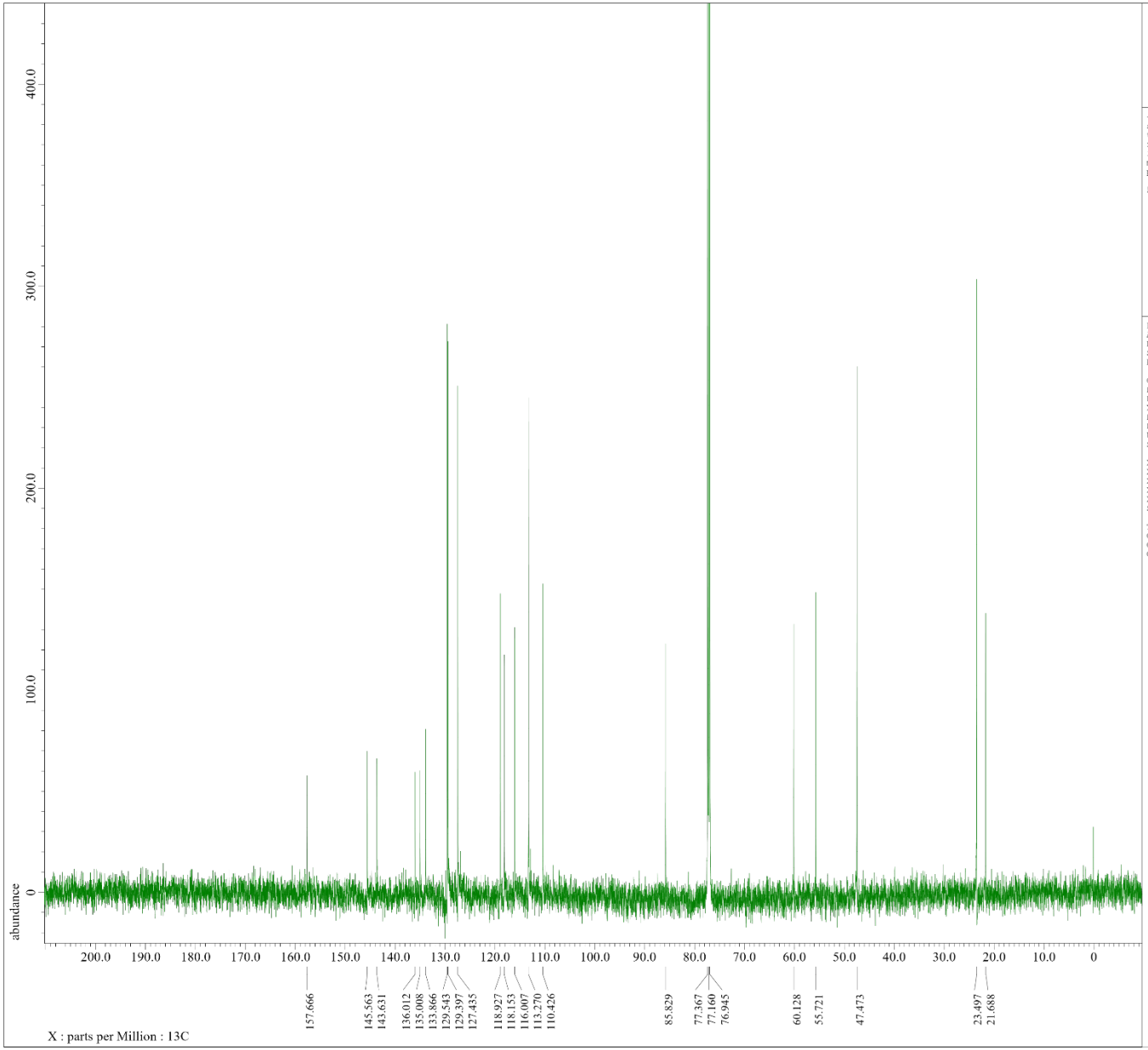


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-123-1-1.jdf
```

```
Filename       = KY-2-123-1-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 28-MAR-2025 18:37:53

Comment        = s2pul
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = 151.73991044[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```


***trans*-4hdg**



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

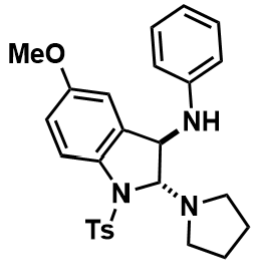
以下に由来:: KY-2-123-1-carbon-2.jdf

Filename = KY-2-123-1-carbon-3.jdf
Author = 德里魔祐
Experiment = s2pul
Solvent = cdcl3
Revision_Time = 24-APR-2025 11:49:53

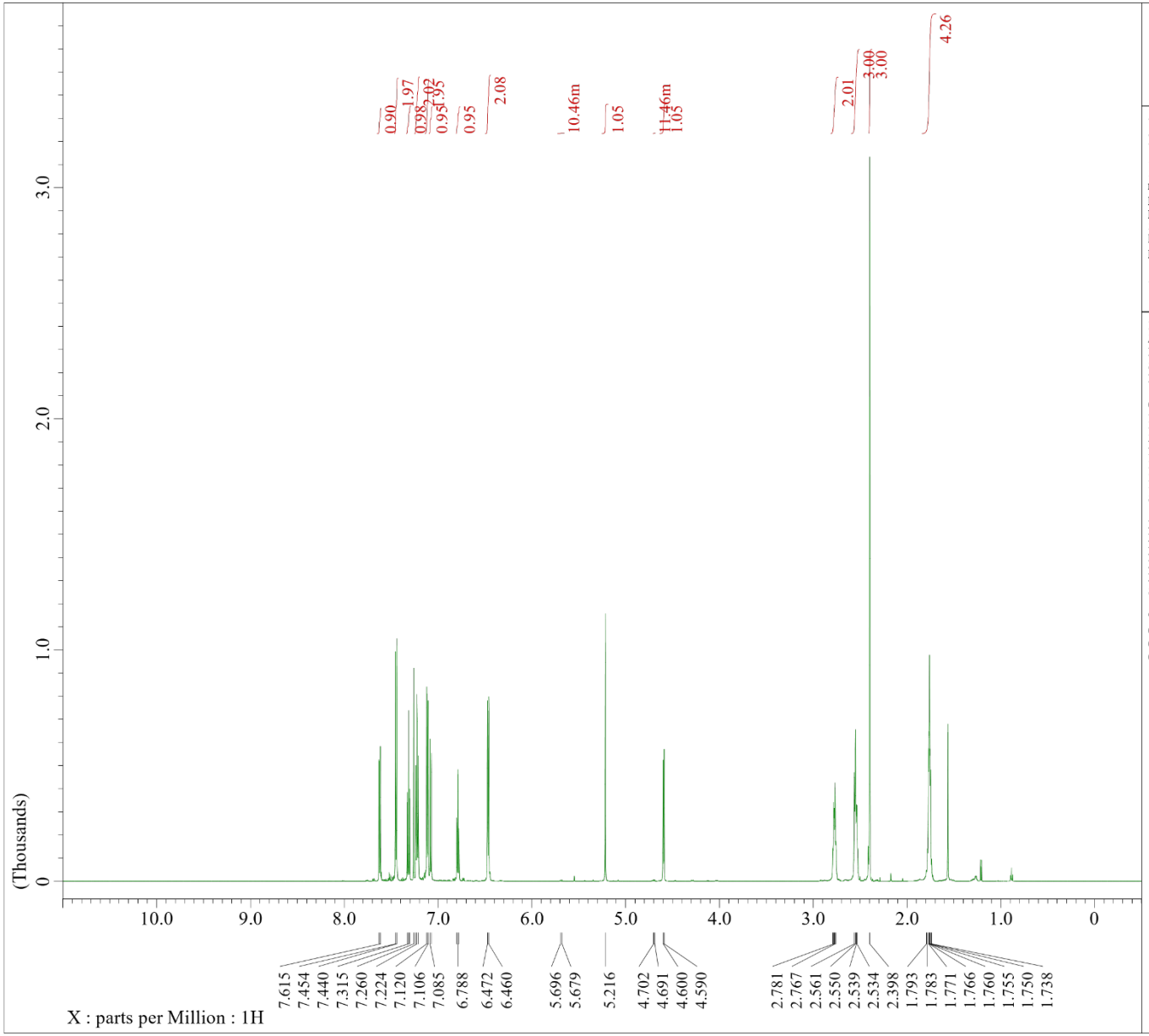
Comment = s2pul
Data Format = 1D COMPLEX
Dim_Size = 32768
X_Domain = 13
Dim Title = 13C
Dim Units = [ppm]
Dimensions = X
Spectrometer = VARIAN_UNITY_NMR

X_Domain = 13C
X_Freq = 150.81013958[MHz]
X_Freq_Flip = FALSE
X_Offset = 16.58911607[kHz]
X_Sweep = 37.87878788[kHz]
Scans = 256

Temp_Get = 00[dC]
Ovj_P0 = 110.32884979[deg]
Ovj_P1 = 0[deg]
Ovj_Pp = 100[%]



***trans*-4hdg**



---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-5.5, 29, 72.53334[%])
reference(7.25492[ppm], 7.26[ppm])
base correct(Akima, 5, 0, FALSE, 3, None, FAL
phase(0, 0, 50[%])

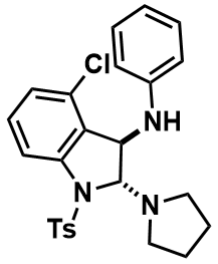
以下に由来:: KY-2-100-7-1.jdf

Filename = KY-2-100-7-2.jdf
Author = Y.Kobori
Experiment = s2pul
Solvent = cdcl3
Revision_Time = 23-MAR-2025 17:11:01

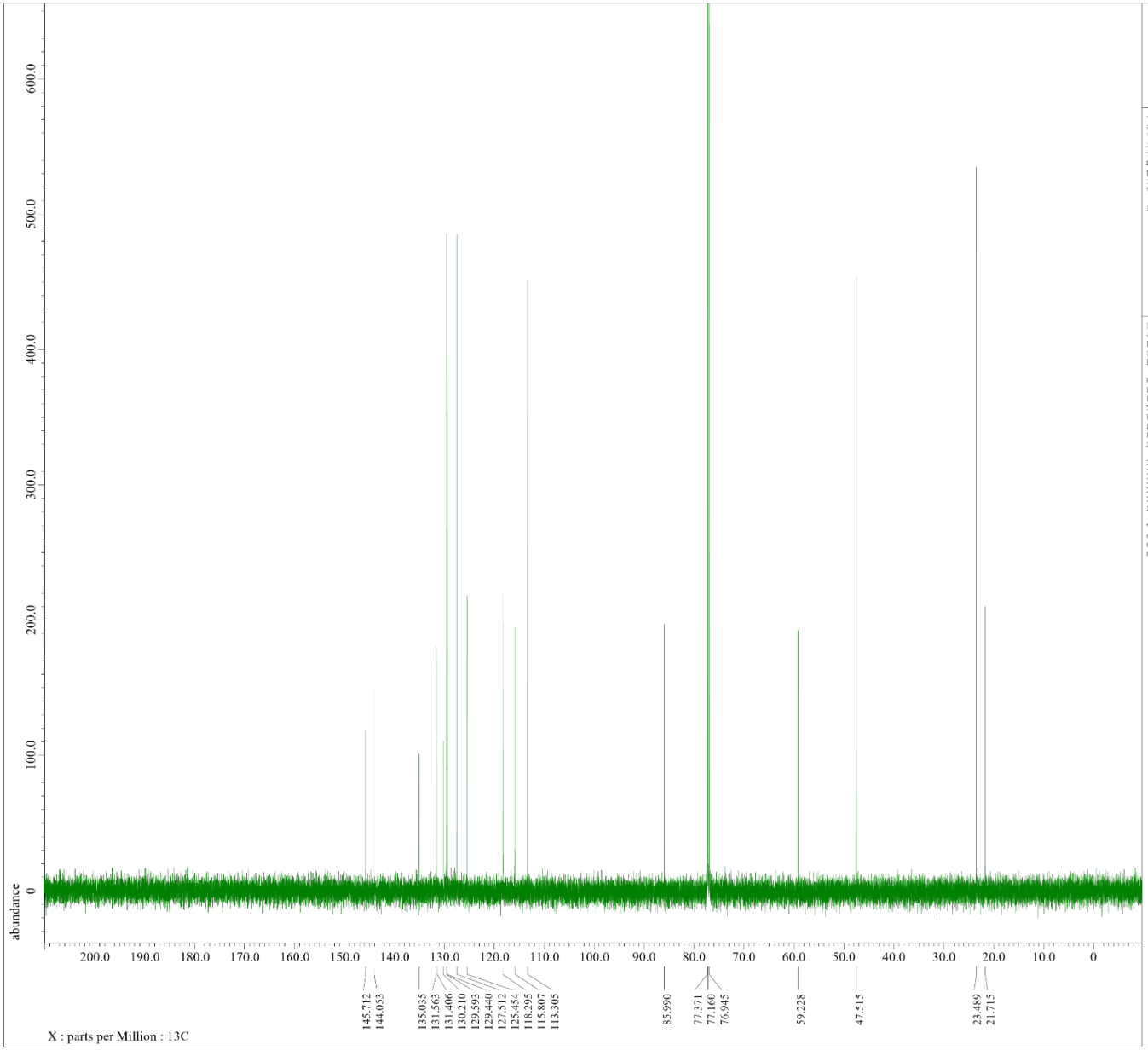
Comment = s2pul
Data_Format = 1D REAL
Dim_Size = 32768
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Spectrometer = VARIAN_UNITY_NMR

X_Domain = 1H
X_Freq = 599.76146205[MHz]
X_Freq_Flip = FALSE
X_Offset = 3.59855331[kHz]
X_Sweep = 9.61538462[kHz]
Scans = 16

Temp_Get = 80[dC]
Ovj_P0 = 157.56140785[deg]
Ovj_P1 = 0[deg]
Ovj_Pp = 100[%]



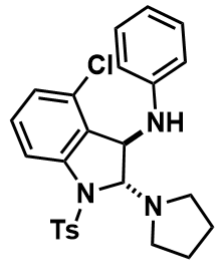
***trans*-4idg**



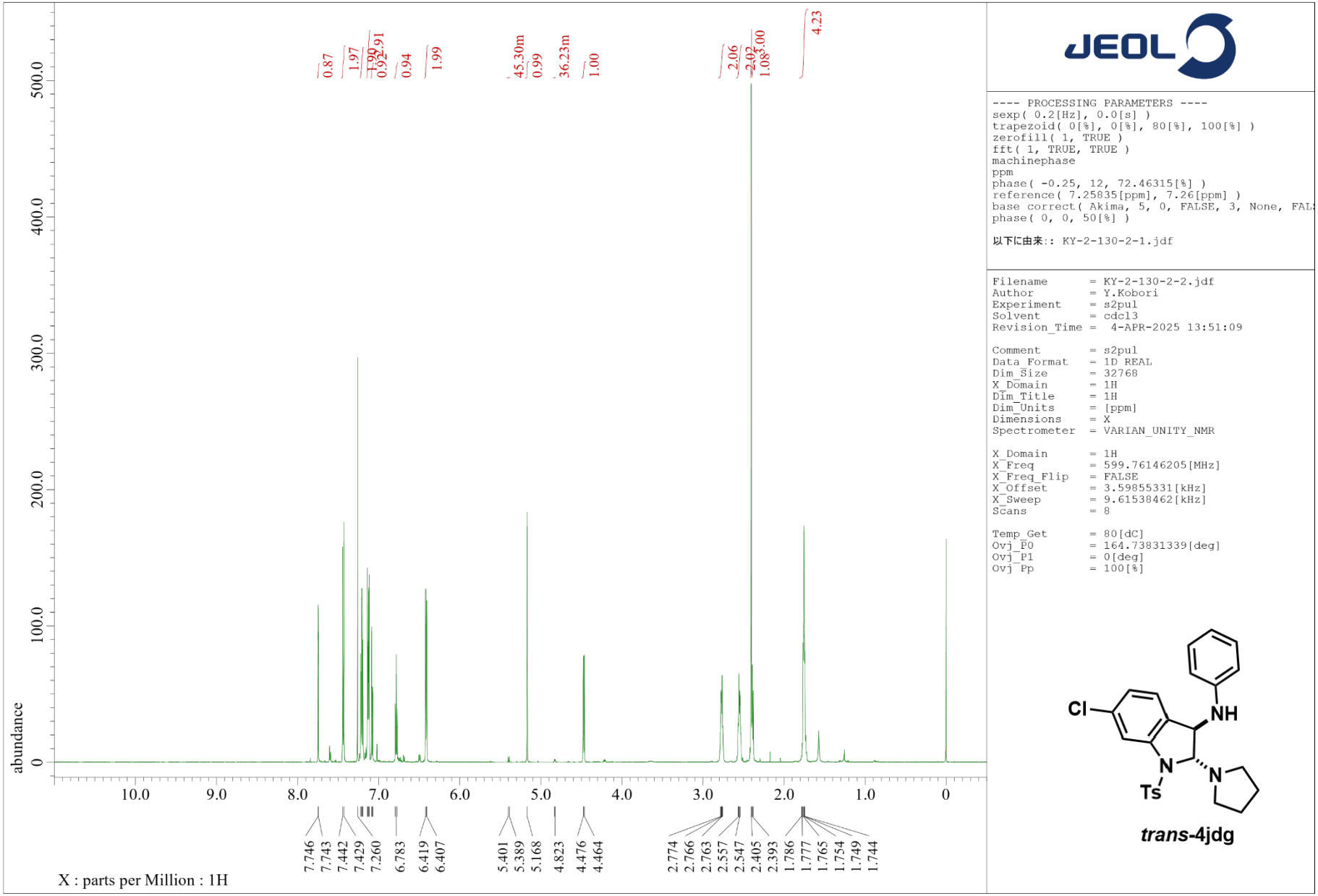
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.1[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.01725[ppm], 77.16[ppm] )
thresh( 1, 2.68655[%], )

以下に由来:: KY-2-100-7-carbon-1.jdf
```

```
Filename        = KY-2-100-7-carbon-2.jdf
Author          = 德里庆祐
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   = 24-APR-2025 11:37:52

Comment         = s2pul
Data Format     = 1D COMPLEX
Dim_Size        = 65536
X_Domain        = 13
DIm_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 13C
X_Freq          = 150.81013958[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 16.58911607[kHz]
X_Sweep         = 37.87878788[kHz]
Scans           = 256

Temp_Get        = 80[dC]
Ovj_Fo          = 87.77150539[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```



***trans*-4idg**

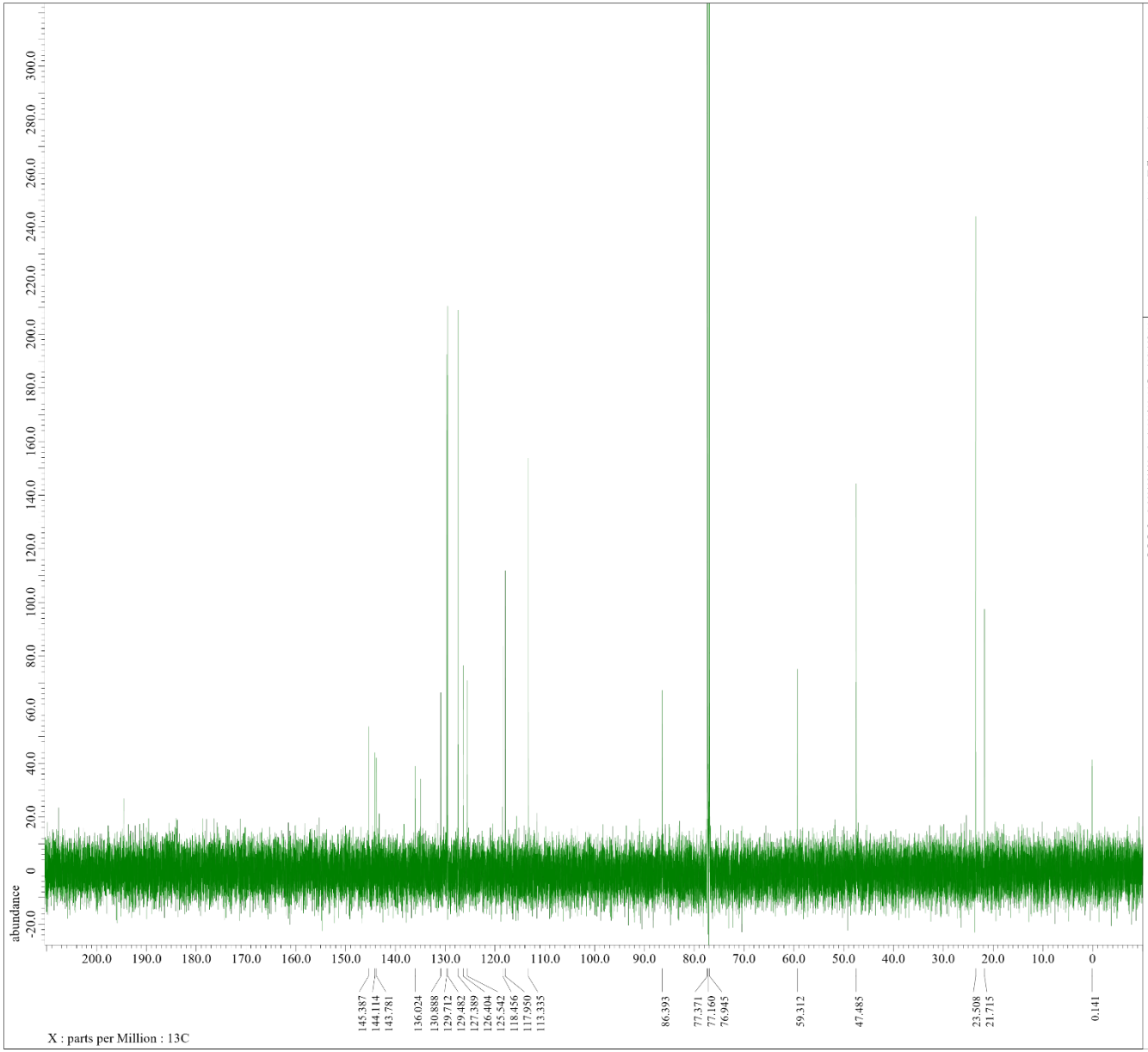


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -0.25, 12, 72.46315[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-130-2-1.jdf
```

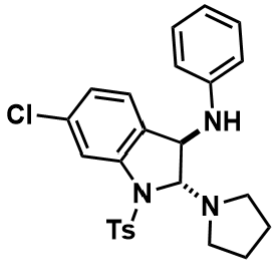
```
Filename        = KY-2-130-2-2.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   =  4-APR-2025 13:51:09

Comment         = s2pul
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 80[dC]
Ovj_P0          = 164.73831339[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```


***trans*-4jdg**

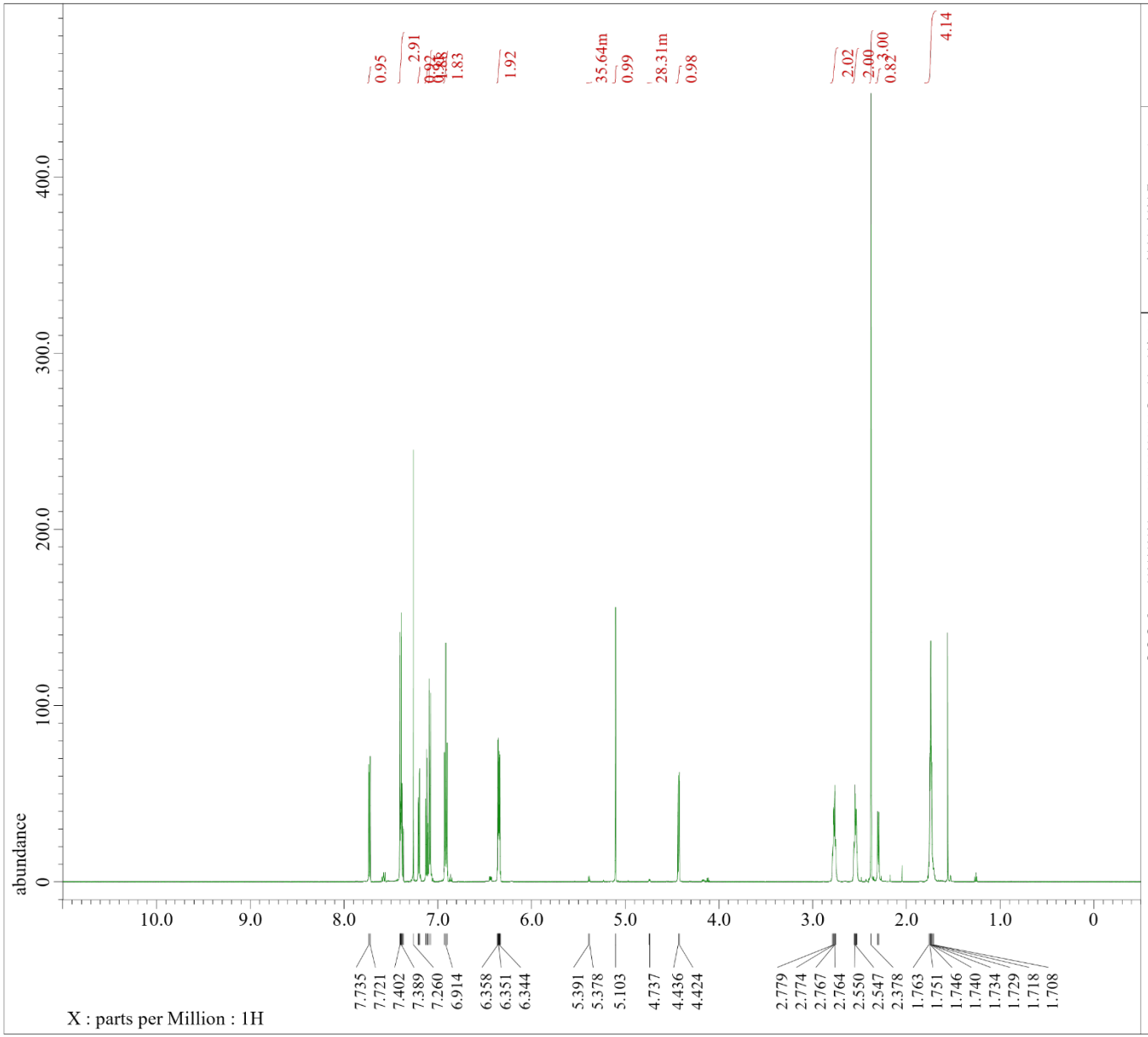



```
---- PROCESSING PARAMETERS ----
SOXH( 0.1[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.05174[ppm], 77.16[ppm] )
reference( 77.11784[ppm], 77.16[ppm] )
thresh( 2.11175[%], 1.76591[%],  )

以下に由来： KY-2-118-1-carbon-1.jdf
```

```
Filename        = KY-2-118-1-carbon-2.jdf
Author          = 徳重慶祐
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   = 24-APR-2025 11:47:45

Comment         = STANDARD PHOSPHORUS PARAMETERS
Data_Format     = 1D COMPLEX
Dim_Size        = 65536
X_Domain        = 13
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 13C
X_Freq          = 150.81013958[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 16.58911607[kHz]
X_Sweep         = 37.87878788[kHz]
Scans           = 256

Temp_Get        = 80[dC]
Ovj_Fo          = 121.06295259[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```

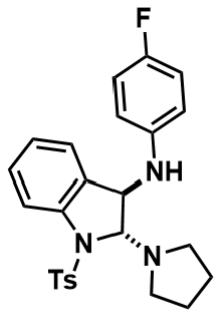


***trans*-4jdg**

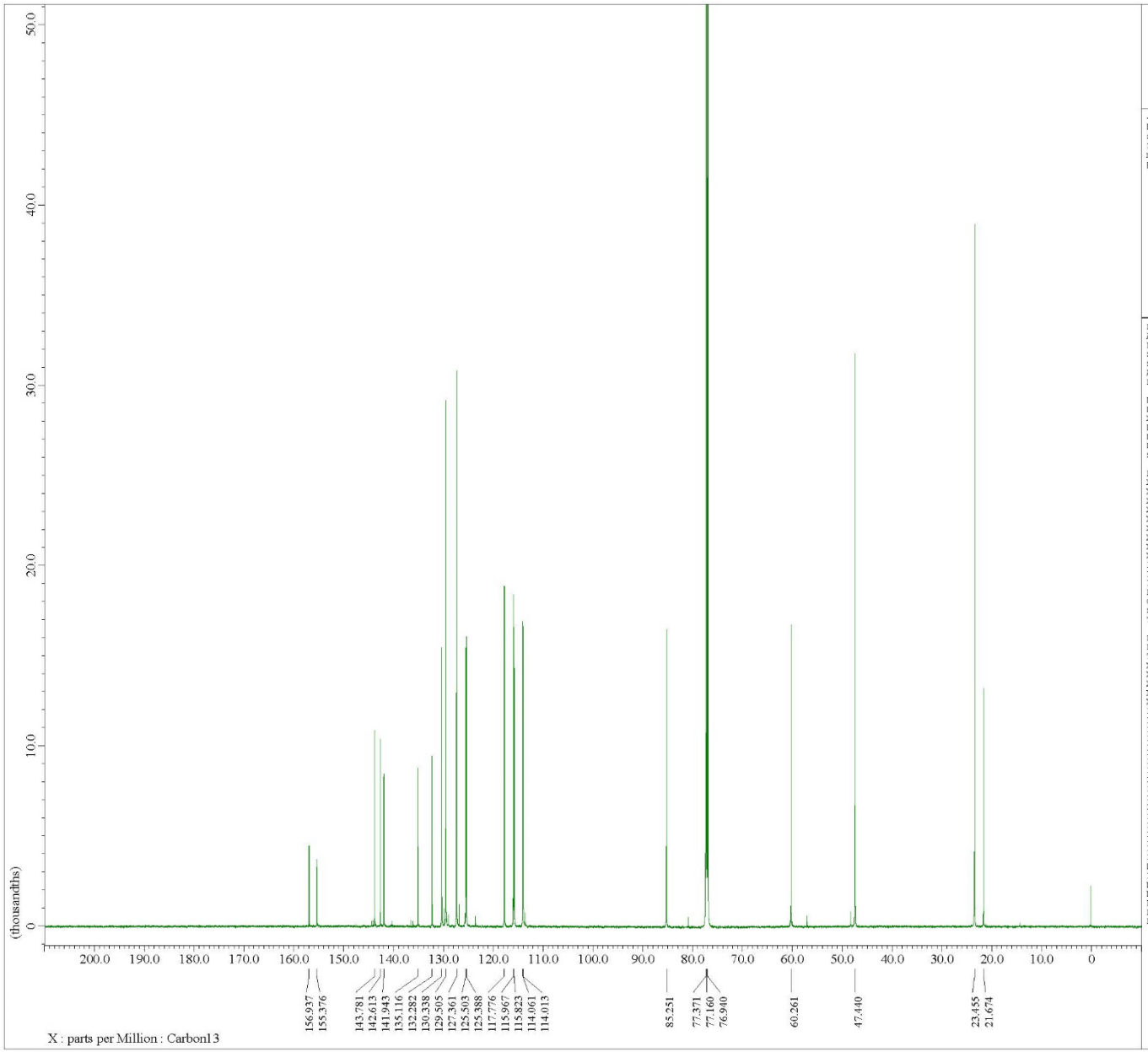



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -5.75, 30, 72.71645[%] )
reference( 7.26[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-036-1-2.jdf
```

```
Filename        = KY-2-036-1-3.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   =  1-APR-2025 15:01:45

Comment         = STANDARD 1H OBSERVE - profile
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146106[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59954467[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 0[dC]
Ovj_P0          = 164.57933919[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```

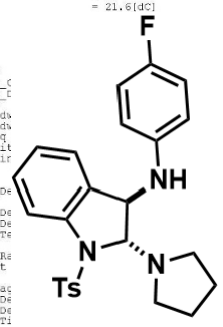


***trans*-4ajg**

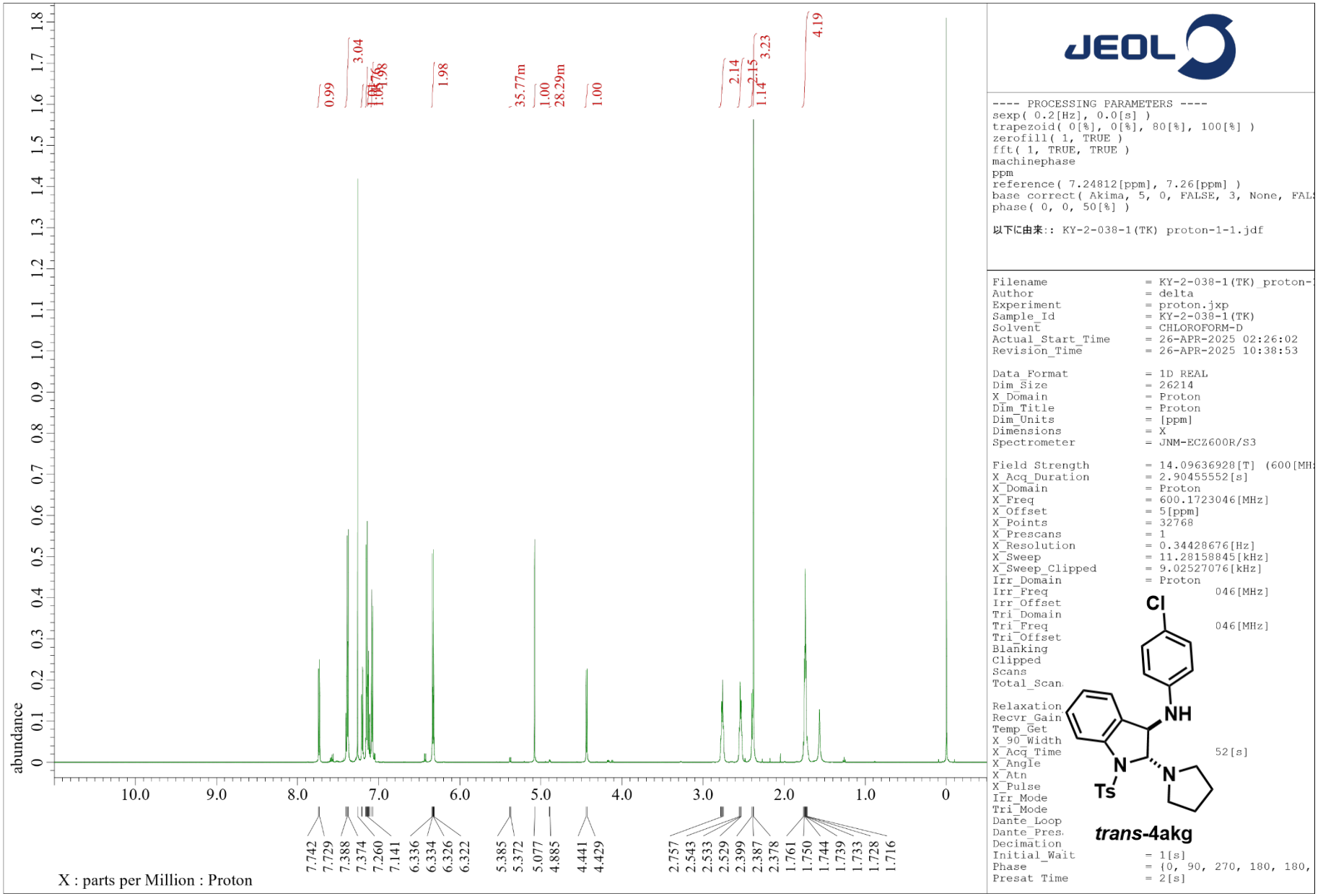


---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm

Filename	= KY-2-036-1(TK)-carbon_carbon-1-2.jdf
Author	= delta
Experiment	= Carbon.jxp
Sample_Id	= KY-2-036-1(TK)-carbon
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-APR-2025 23:16:46
Revision_Time	= 26-APR-2025 09:01:20
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09638928[T] (600[MHz])
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15.8[us]
Clipped	= FALSE
Scans	= 4000
Total_Scans	= 4000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Set	= 21.6[dC]
X_90_Width	
X_Acq_Time	
X_Angle	
X_Atn	
X_Pulse	
Irr_Atn_Dec	
Irr_Atn_Dec_(	
Irr_Atn_Dec_[	
Irr_Atn_Noe	
Irr_Dec_Bandw	
Irr_Dec_Bandw	
Irr_Dec_Freq	
Irr_Dec_Merit	
Irr_Decouplir	
Irr_Noe	
Irr_Noise	
Irr_Offset_De	
Irr_Pwidth	
Irr_Pwidth_De	
Irr_Pwidth_De	
Irr_Pwidth_Ts	
Irr_Wurst	
Declination_Ra	
Initial_Wait	
Noe_Time	
Noe_Time_Flag	
Relaxation_De	
Relaxation_De	
Repetition_Ti	



***trans*-4ajg**

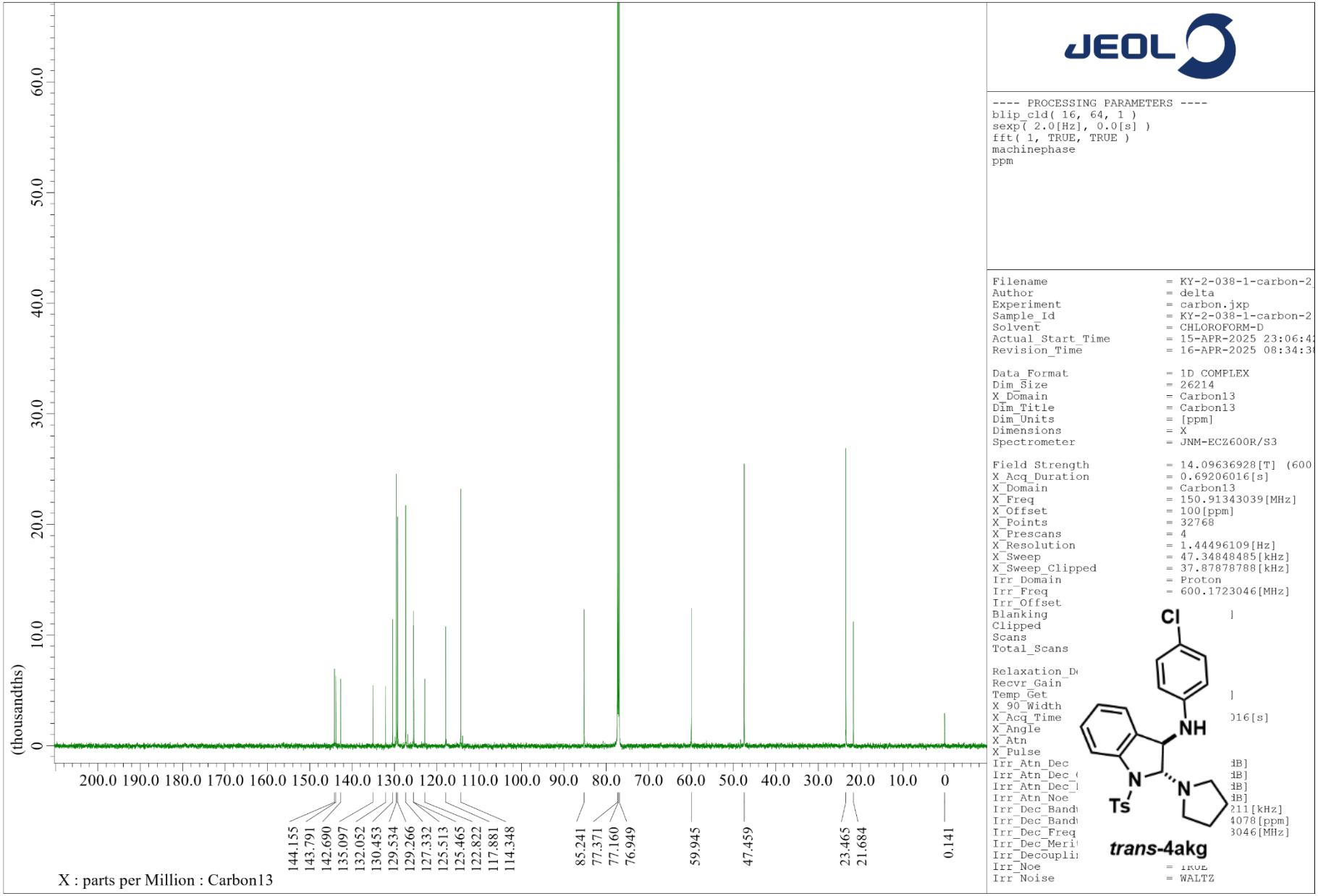


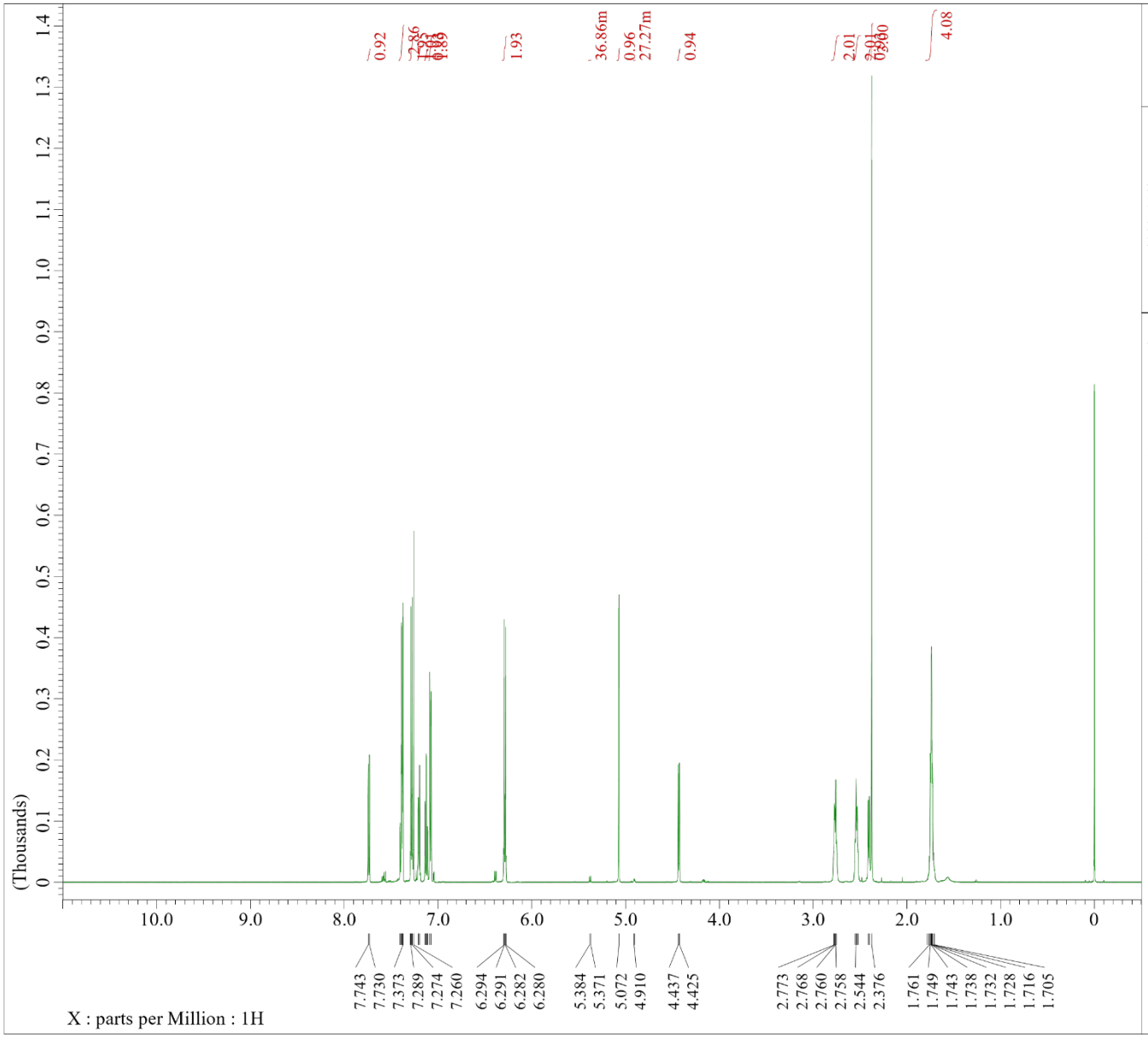
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.24812[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-038-1(TK) proton-1-1.jdf
```

```
Filename              = KY-2-038-1(TK)_proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = KY-2-038-1(TK)
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 26-APR-2025 02:26:02
Revision_Time         = 26-APR-2025 10:38:53

Data_Format           = 1D REAL
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[MH
X_Acq_Duration        = 2.90455552[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.34428676[Hz]
X_Sweep               = 11.28158845[kHz]
X_Sweep_Clipped       = 9.02527076[kHz]
Irr_Domain            = Proton
Irr_Freq                        046[MHz]
Irr_Offset
Tri_Domain
Tri_Freq                        046[MHz]
Tri_Offset
Blanking
Clipped
Scans
Total_Scan

Relaxation
Recvr_Gain
Temp_Get
X_90_Width
X_Acq_Time                      52[s]
X_Angle
X_Atn
X_Pulse
Irr_Mode
Tri_Mode
Dante_Loop
Dante_Pres
Decimation
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180,
Presat_Time           = 2[s]
```

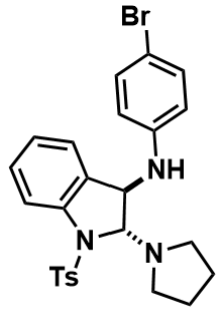

***trans*-4akg**


(thousandths)
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
144.155
143.791
142.690
135.097
132.052
130.453
129.534
129.266
127.332
125.513
125.465
122.822
117.881
114.348
85.241
77.371
77.160
76.949
59.945
47.459
23.465
21.684
0.141
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = KY-2-038-1-carbon-2
Author = delta
Experiment = carbon.jxp
Sample_Id = KY-2-038-1-carbon-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-APR-2025 23:06:4
Revision_Time = 16-APR-2025 08:34:3
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset
Blanking]
Clipped
Scans
Total_Scans
Relaxation_D
Recvr_Gain
Temp_Get]
X_90_Width
X_Acq_Time 016[s]
X_Angle
X_Atn
X_Pulse
Irr_Atn_Dec dB]
Irr_Atn_Dec_ dB]
Irr_Atn_Dec_ dB]
Irr_Atn_Noe dB]
Irr_Dec_Band 211[kHz]
Irr_Dec_Band 4078[ppm]
Irr_Dec_Freq 3046[MHz]
Irr_Dec_Meri
Irr_Decoupli
Irr_Noe = TRUE
Irr_Noise = WALTZ
Cl
NH
N
N
Ts
trans-4akg

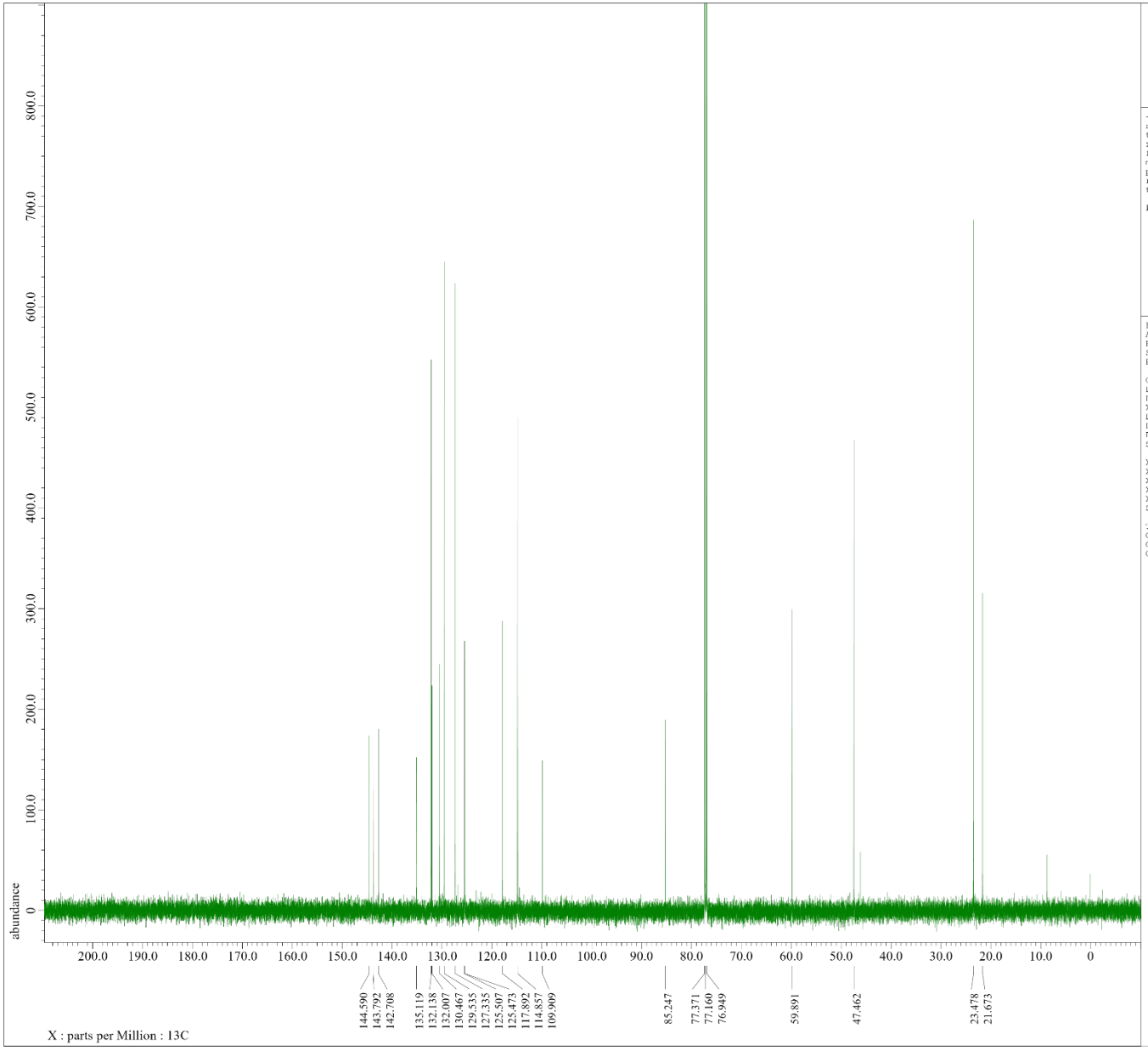



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-139-1-2.jdf
```

```
Filename        = KY-2-139-1-3.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   = 10-APR-2025 16:08:21

Comment         = ST-462-2
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 80[dC]
Ovj_P0          = 157.83617421[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```



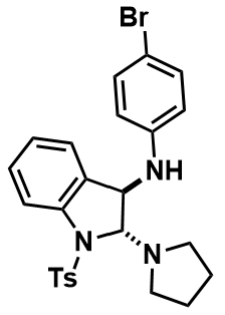
***trans*-4alg**



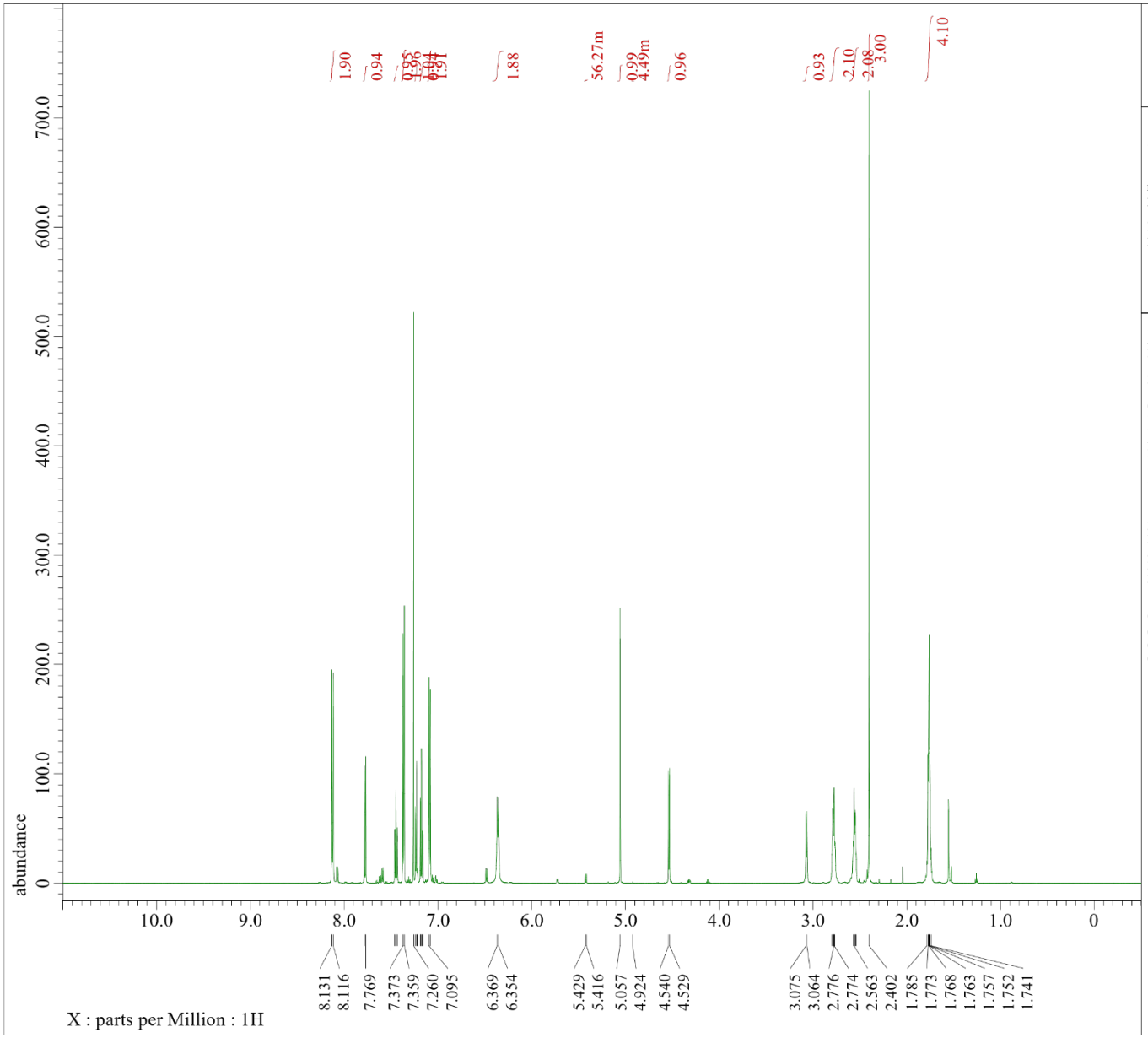
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.1[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.02108[ppm], 77.16[ppm] )
thresh( 6.58832[%], 1,  )

以下に由来:: KY-2-044-1ver.2-carbon-1.jdf
```

```
Filename       = KY-2-044-1ver.2-carbon-2.jdf
Author         = 徳重慶祐
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 24-APR-2025 11:34:12

Comment        = s2pul
Data Format    = 1D COMPLEX
Dim_Size       = 65536
X_Domain       = 13
Dim Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 13C
X_Freq         = 150.81013958[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 16.58911607[kHz]
X_Sweep        = 37.67878788[kHz]
Scans          = 256

Temp Got       = 80[dC]
Ovj_P0         = 97.83109978[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```

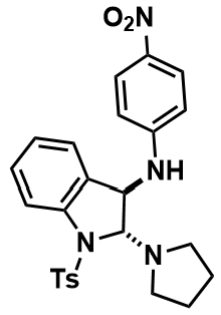


***trans*-4alg**

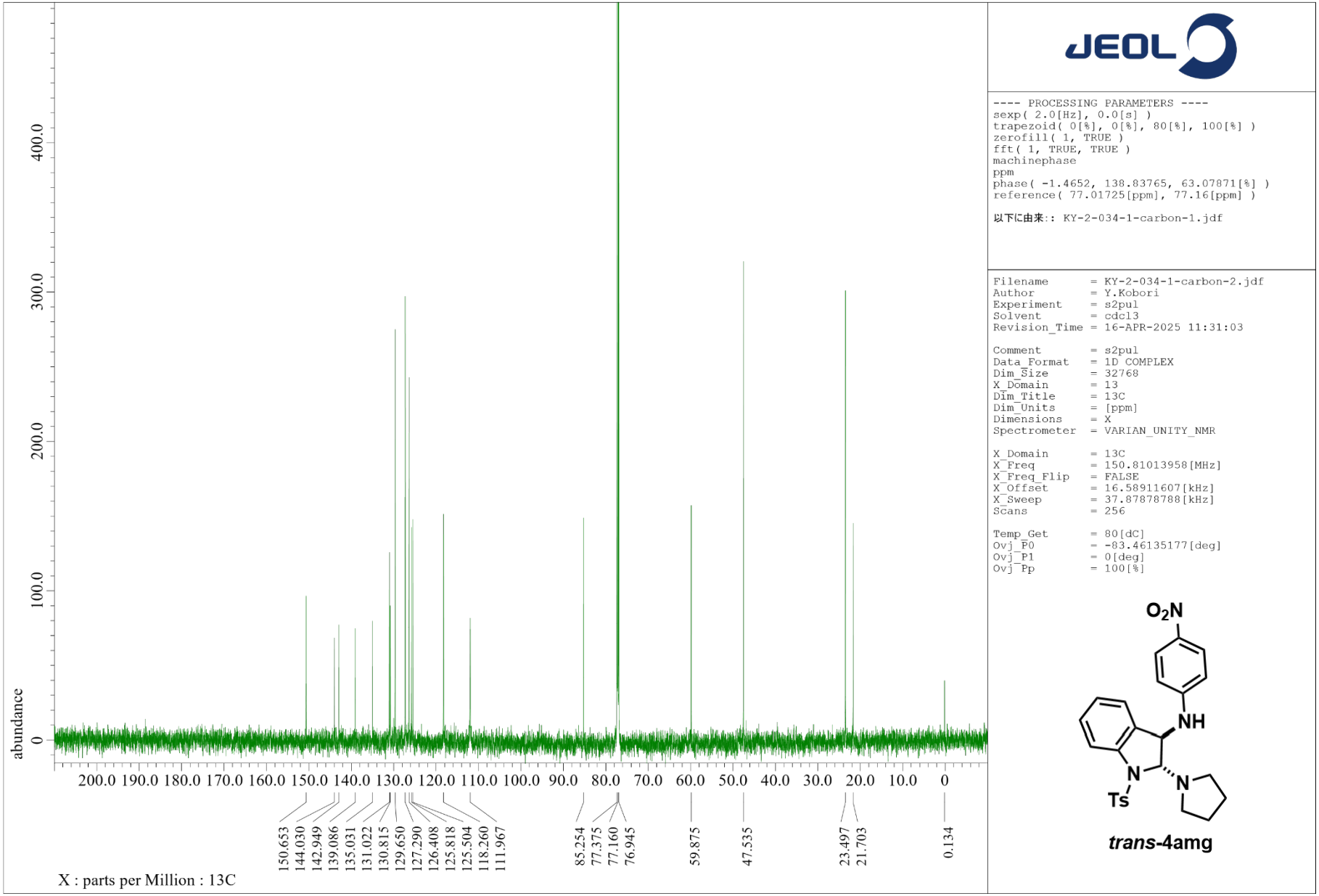



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-034-1-3.jdf
```

```
Filename        = KY-2-034-1-4.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   =  4-APR-2025 18:24:55

Comment         = STANDARD 1H OBSERVE - profile
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 0[dC]
Ovj_P0          = 73.05489674[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```



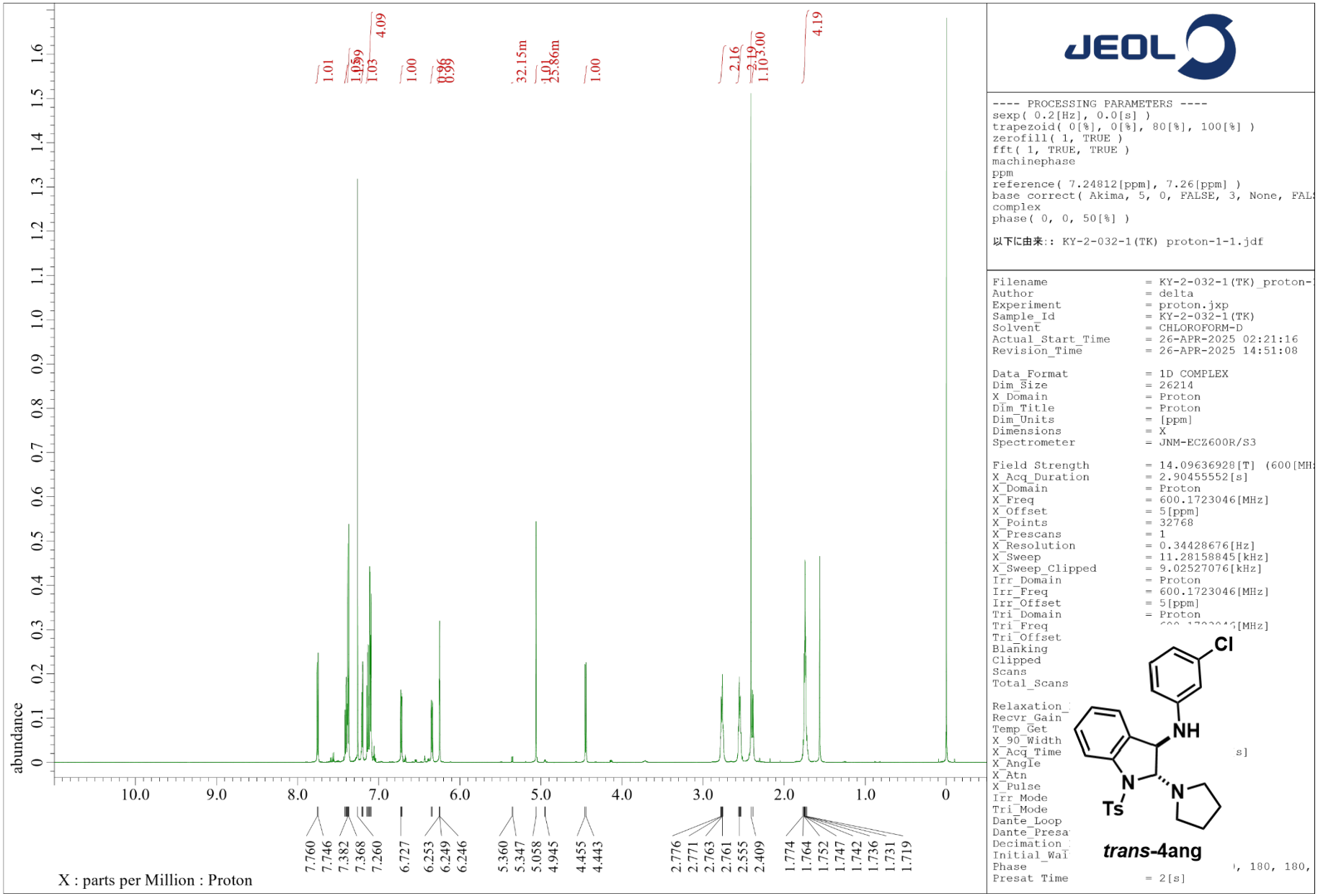
***trans*-4amg**




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -1.4652, 138.83765, 63.07871[%] )
reference( 77.01725[ppm], 77.16[ppm] )

以下に由来:: KY-2-034-1-carbon-1.jdf
```

```
Filename       = KY-2-034-1-carbon-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 16-APR-2025 11:31:03

Comment        = s2pul
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
X_Domain       = 13
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 13C
X_Freq         = 150.81013958[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 16.58911607[kHz]
X_Sweep        = 37.87878788[kHz]
Scans          = 256

Temp_Get       = 80[dC]
Ovj_P0         = -83.46135177[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```


***trans*-4amg**

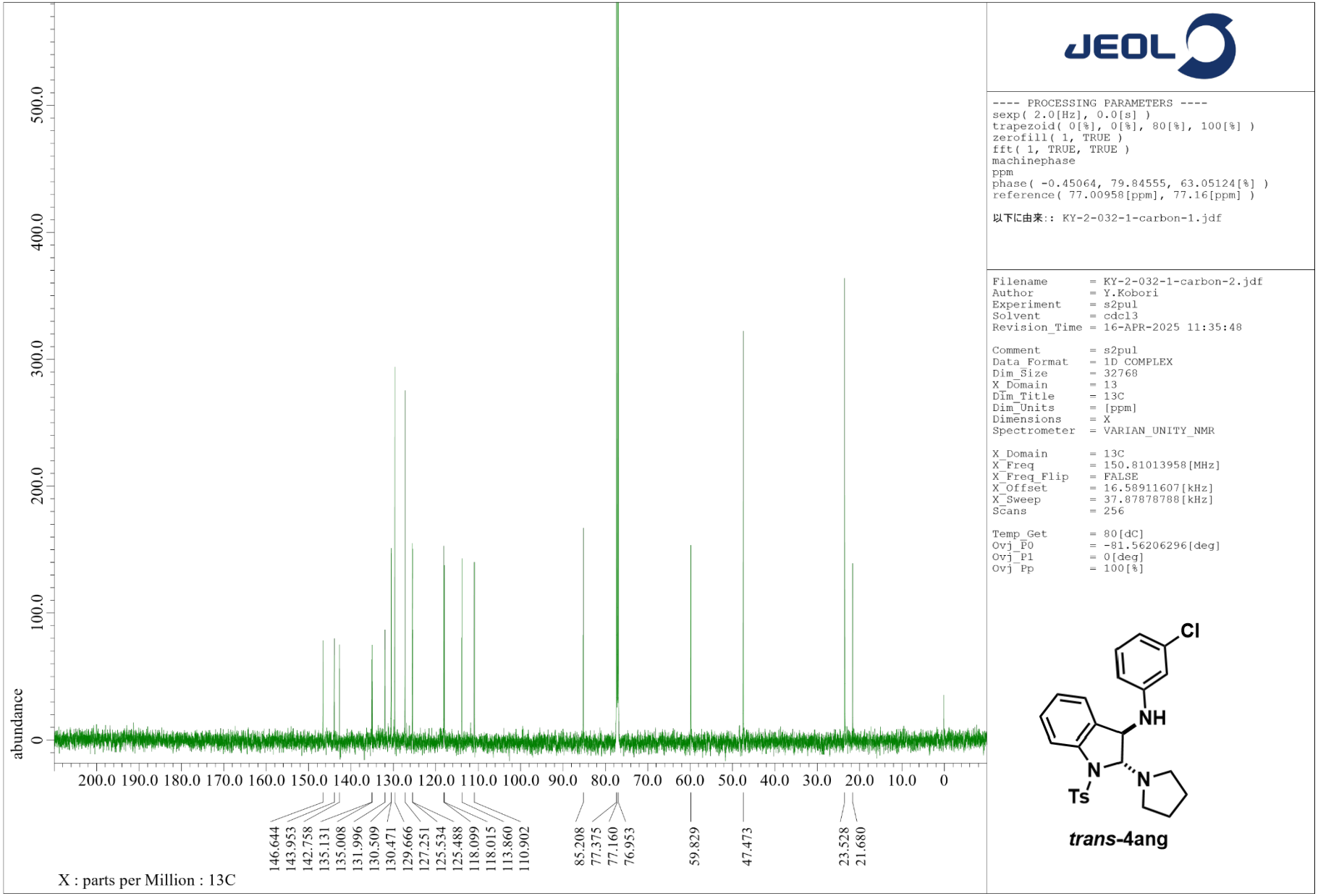


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.24812[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
complex
phase( 0, 0, 50[%] )

以下に由来:: KY-2-032-1(TK) proton-1-1.jdf
```

```
Filename                = KY-2-032-1(TK)_proton-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = KY-2-032-1(TK)
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 26-APR-2025 02:21:16
Revision_Time           = 26-APR-2025 14:51:08

Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (600[MH
X_Acq_Duration          = 2.90455552[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 32768
X_Prescans              = 1
X_Resolution            = 0.34428676[Hz]
X_Sweep                 = 11.28158845[kHz]
X_Sweep_Clipped         = 9.02527076[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                =  [MHz]
Tri_Offset
Blanking
Clipped
Scans
Total_Scans

Relaxation_
Recvr_Gain
Temp_Get
X_90_Width
X_Acq_Time                                  s]
X_Angle
X_Atn
X_Pulse
Irr_Mode
Tri_Mode
Dante_Loop
Dante_Presa
Decimation_
Initial_Wai
Phase                                       , 180, 180,
Presat_Time             = 2[s]
```

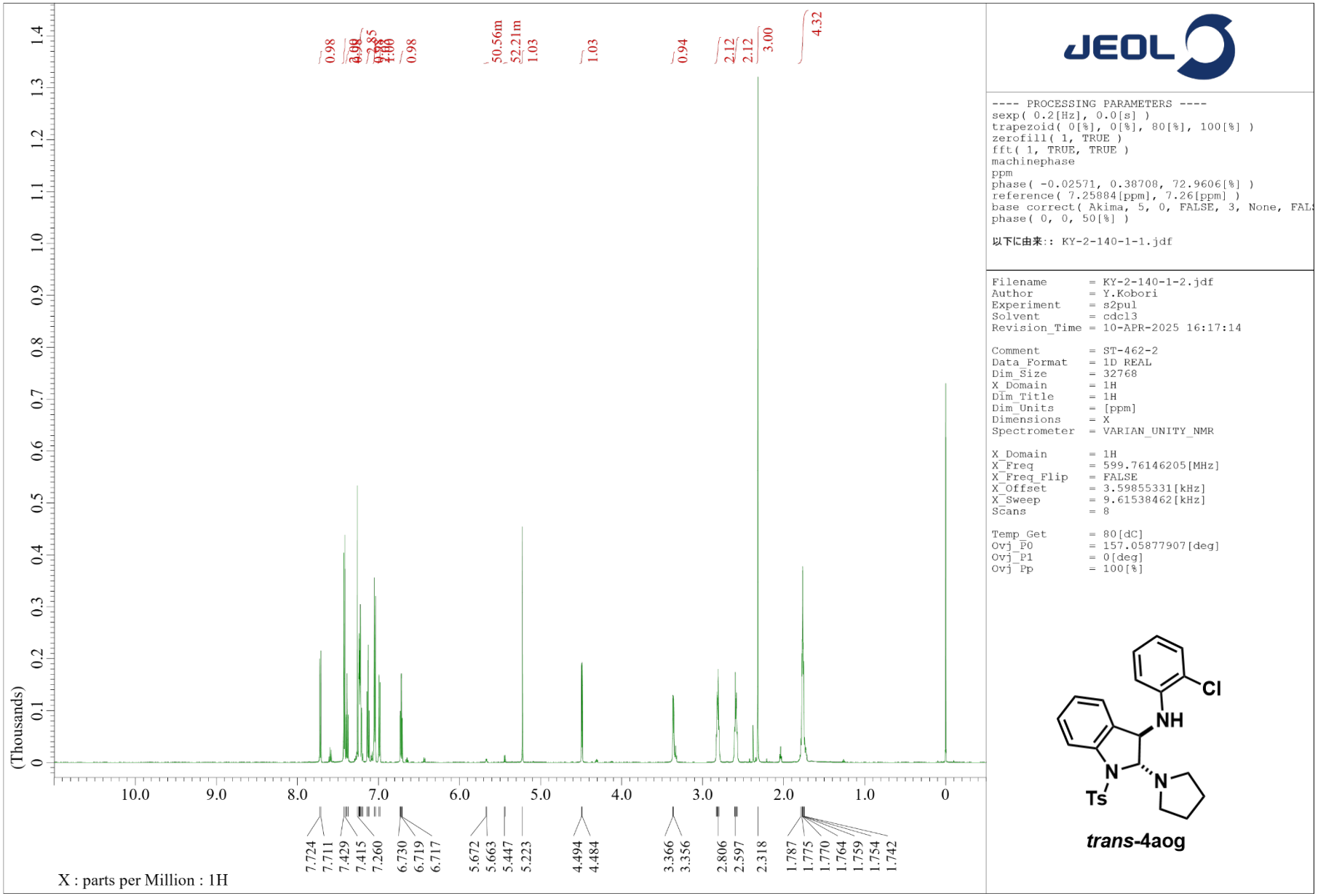

***trans*-4ang**




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -0.45064, 79.84555, 63.05124[%] )
reference( 77.00958[ppm], 77.16[ppm] )

以下に由来:: KY-2-032-1-carbon-1.jdf
```

```
Filename       = KY-2-032-1-carbon-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 16-APR-2025 11:35:48

Comment        = s2pul
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
X_Domain       = 13
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 13C
X_Freq         = 150.81013958[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 16.58911607[kHz]
X_Sweep        = 37.87878788[kHz]
Scans          = 256

Temp_Get       = 80[dC]
Ovj_P0         = -81.56206296[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```

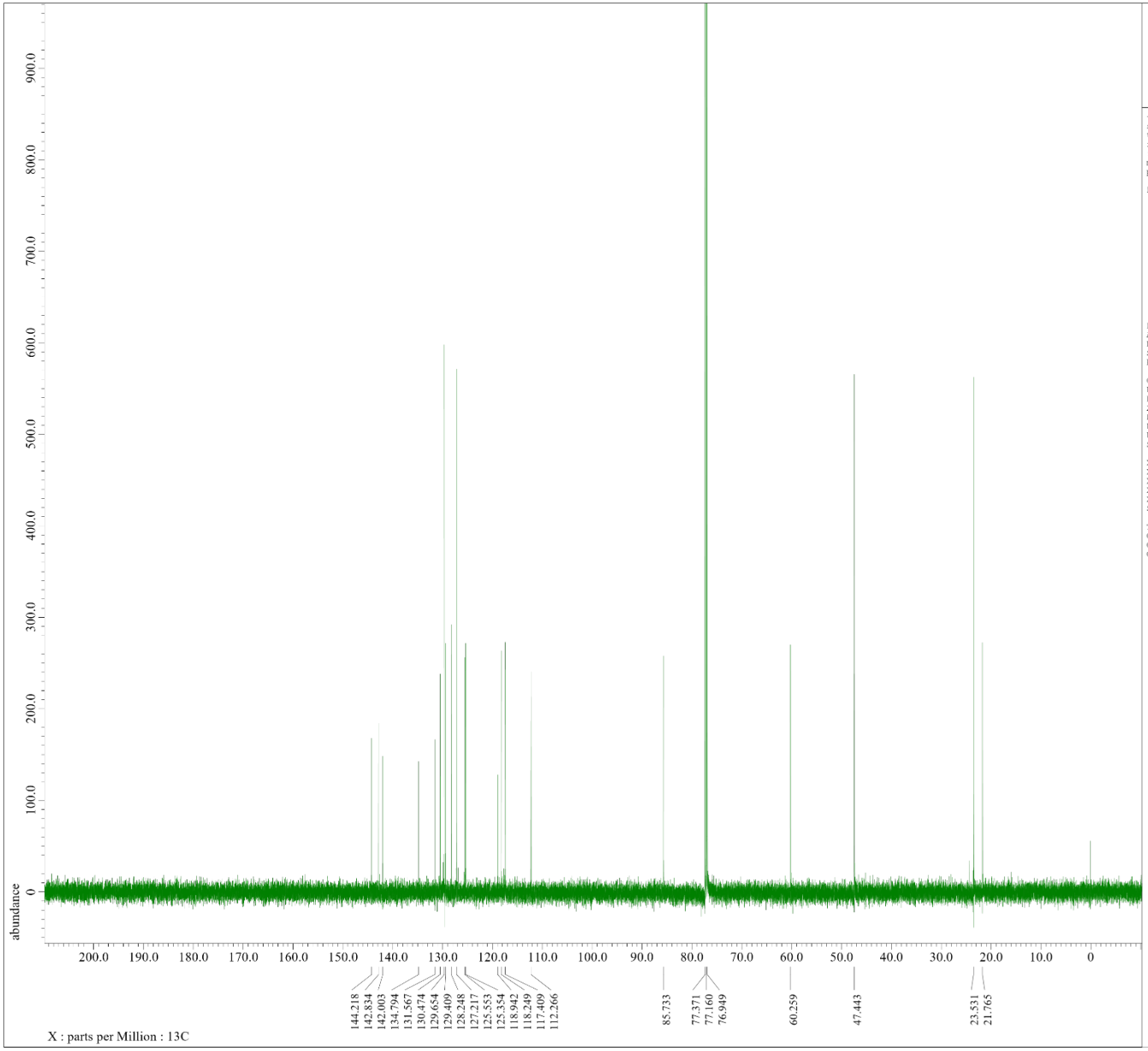

***trans*-4ang**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -0.02571, 0.38708, 72.9606[%] )
reference( 7.25884[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-140-1-1.jdf
```

```
Filename        = KY-2-140-1-2.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   = 10-APR-2025 16:17:14

Comment         = ST-462-2
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 80[dC]
Ovj_P0          = 157.05877907[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```


***trans*-4aog**



---- PROCESSING PARAMETERS ----
sexp(0.1[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm

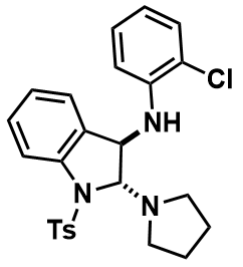
以下に由来:: KY-2-140-1-carbon-1.jdf

Filename = KY-2-140-1-carbon-2.jdf
Author = 徳重慶祐
Experiment = s2pul
Solvent = cdcl3
Revision_Time = 24-APR-2025 12:08:43

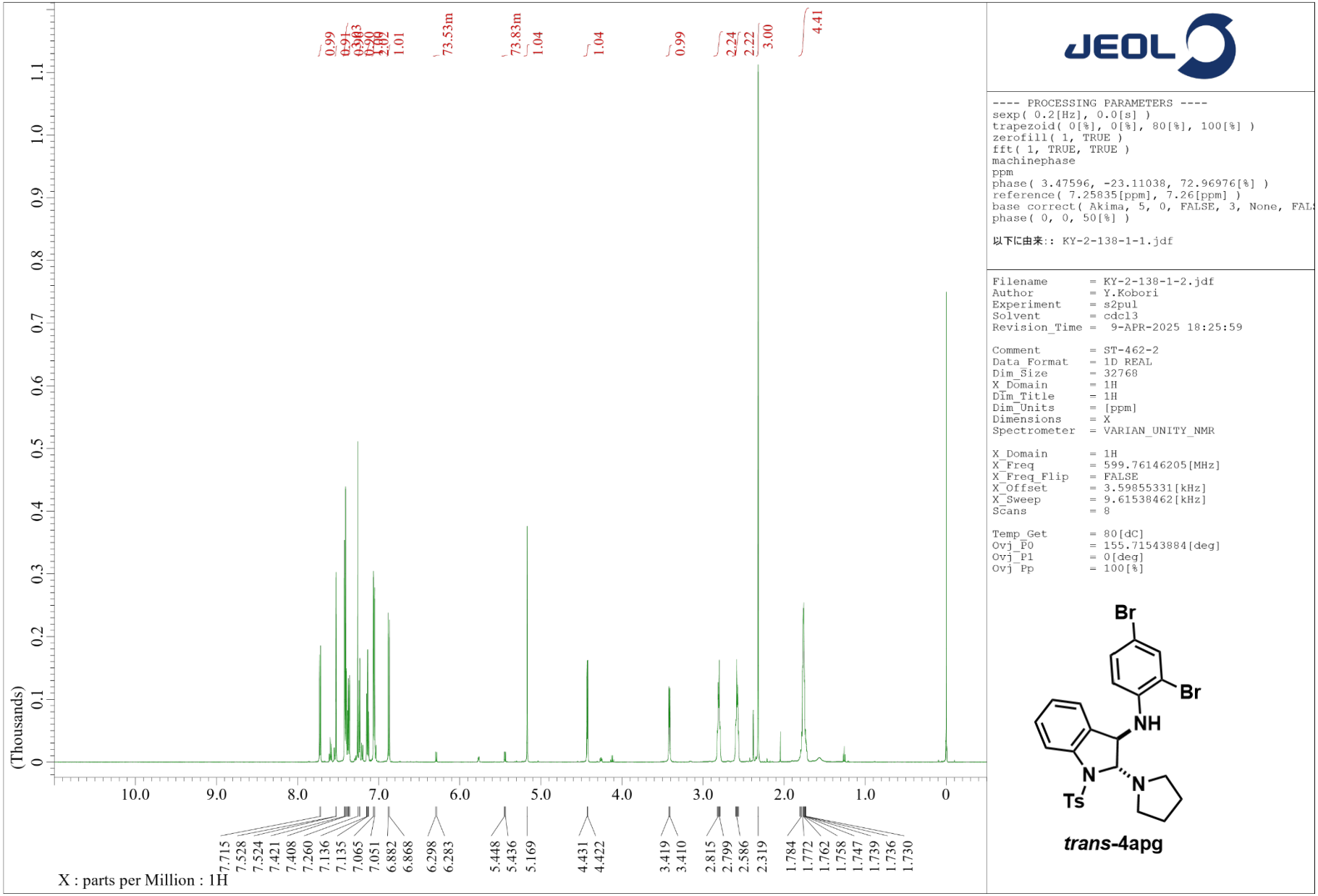
Comment = STANDARD 1H OBSERVE - proiile
Data_Format = 1D COMPLEX
Dim_Size = 65536
X_Domain = 13
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Spectrometer = VARIAN_UNITY_NMR

X_Domain = 13C
X_Freq = 150.81013958[MHz]
X_Freq_Flip = FALSE
X_Offset = 16.58911607[kHz]
X_Sweep = 37.87878788[kHz]
SCans = 256

Temp_Get = 00[dC]
Ovj_P0 = 110.96675427[deg]
Ovj_P1 = 0[deg]
Ovj_Pp = 100[%]



***trans*-4aog**

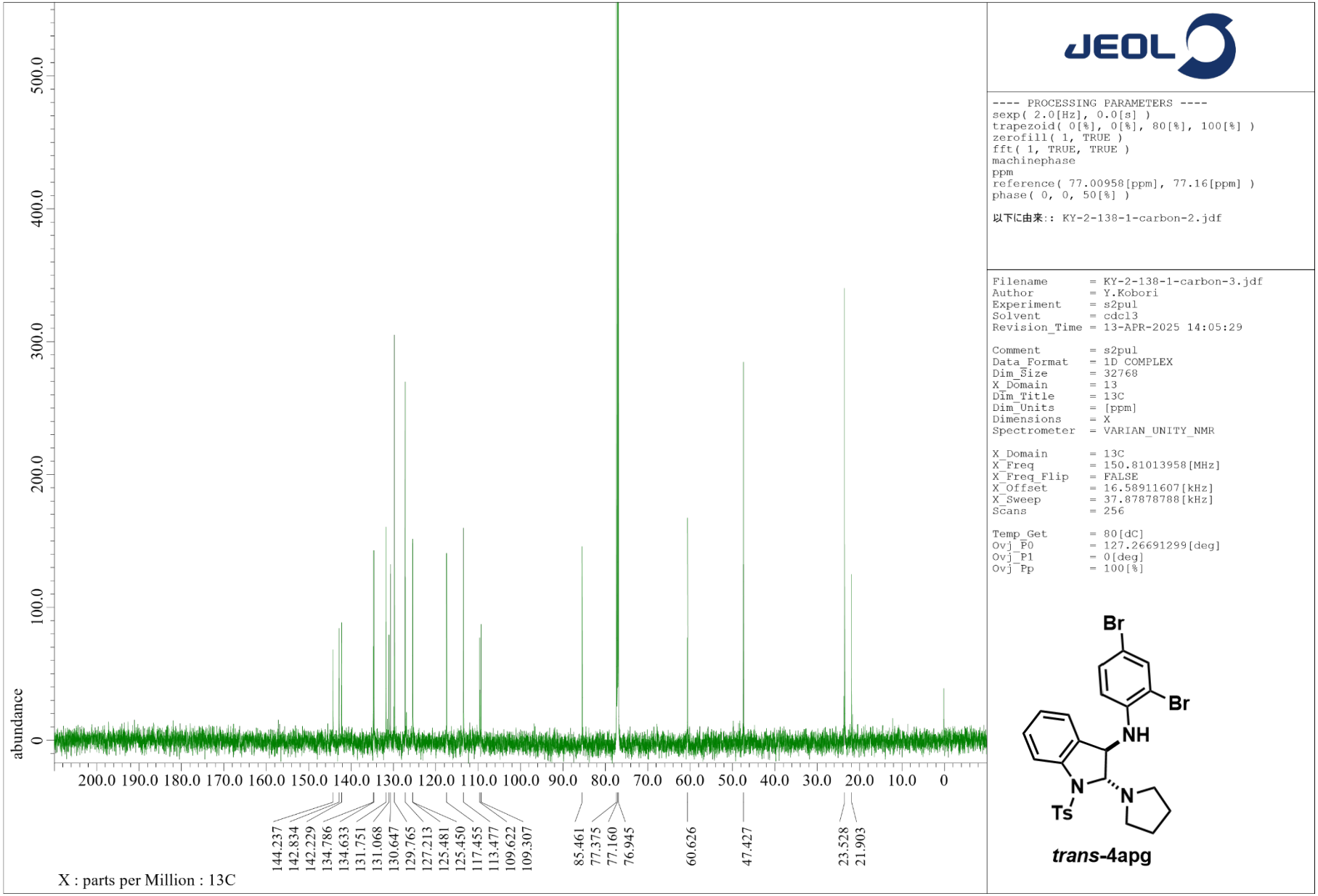


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 3.47596, -23.11038, 72.96976[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-138-1-1.jdf
```

```
Filename        = KY-2-138-1-2.jdf
Author          = Y.Kobori
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   =  9-APR-2025 18:25:59

Comment         = ST-462-2
Data_Format     = 1D REAL
Dim_Size        = 32768
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 1H
X_Freq          = 599.76146205[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 3.59855331[kHz]
X_Sweep         = 9.61538462[kHz]
Scans           = 8

Temp_Get        = 80[dC]
Ovj_P0          = 155.71543884[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```


***trans*-4apg**

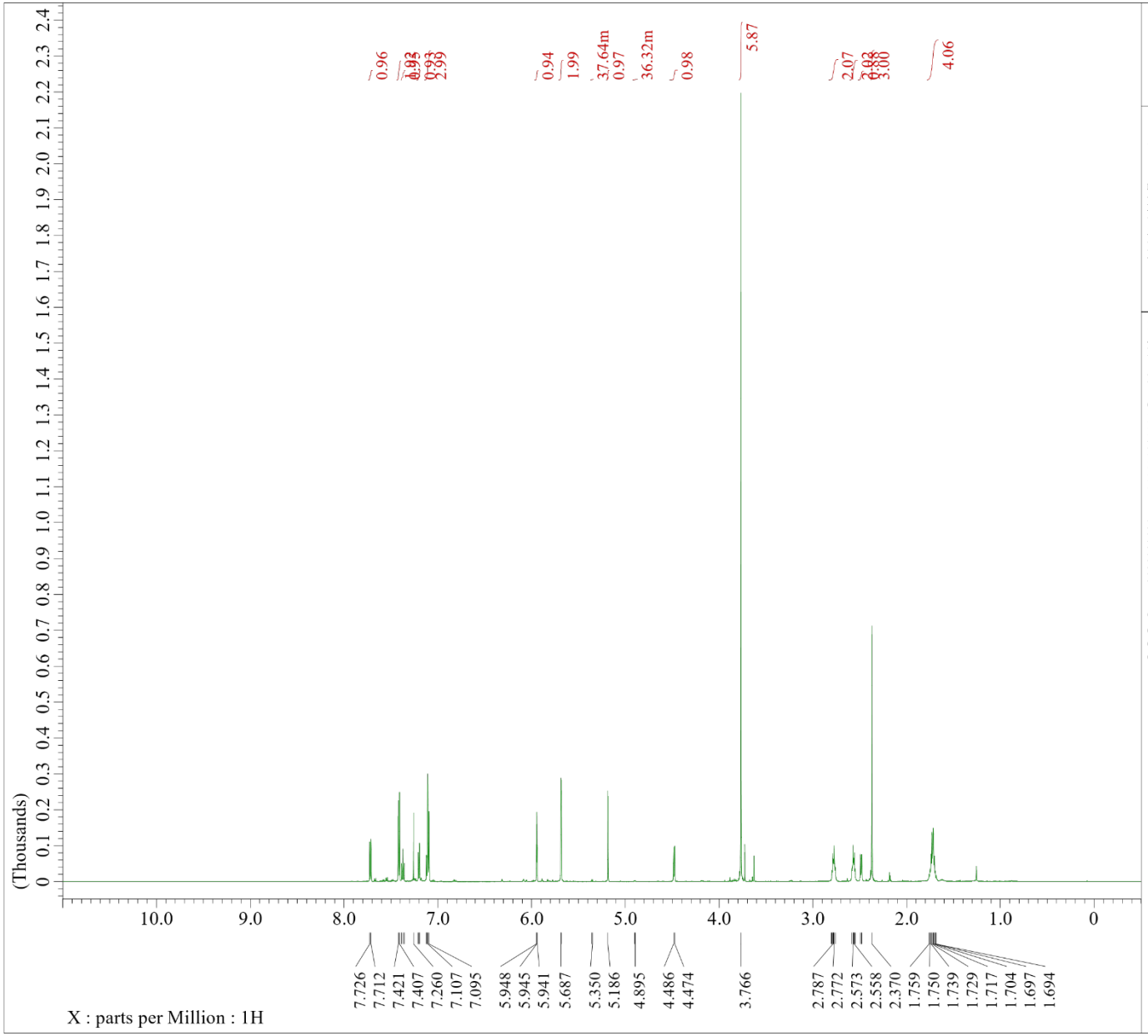


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.00958[ppm], 77.16[ppm] )
phase( 0, 0, 50[%] )

以下に由来:: KY-2-138-1-carbon-2.jdf
```

```
Filename       = KY-2-138-1-carbon-3.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 13-APR-2025 14:05:29

Comment        = s2pul
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
X_Domain       = 13
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 13C
X_Freq         = 150.81013958[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 16.58911607[kHz]
X_Sweep        = 37.87878788[kHz]
Scans          = 256

Temp_Get       = 80[dC]
Ovj_P0         = 127.26691299[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```

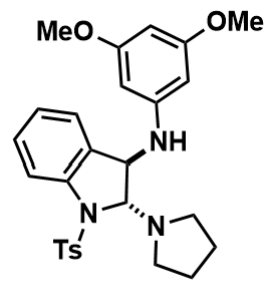

***trans*-4apg**



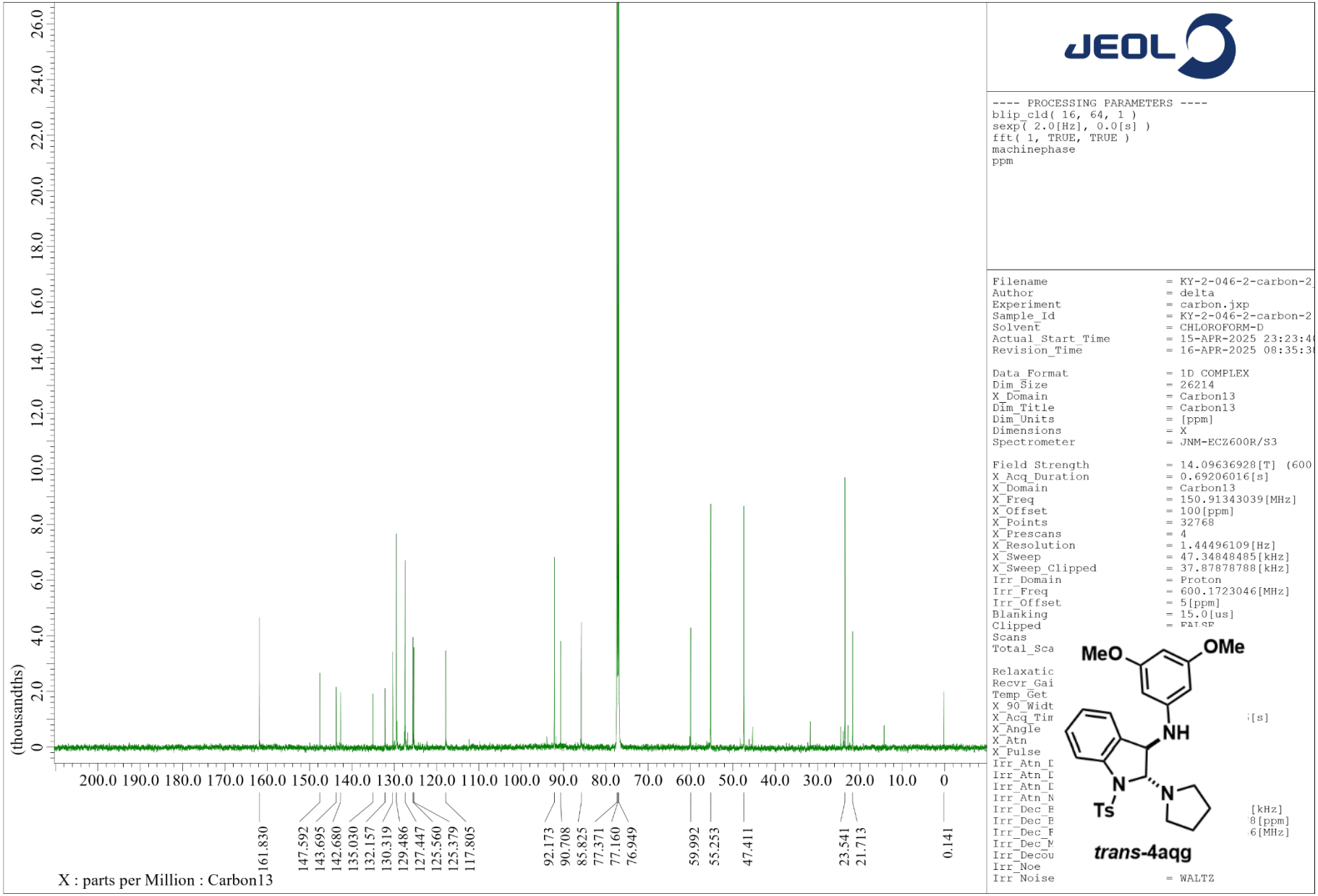
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 0.34697, -22.26798, 63.92407[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FALS
phase( 0, 0, 50[%] )

以下に由来:: KY-2-046-5-2.jdf
```

```
Filename       = KY-2-046-5-3.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  =  1-APR-2025 14:38:45

Comment        = new experiment
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 0[dC]
Ovj_P0         = 151.23542418[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```



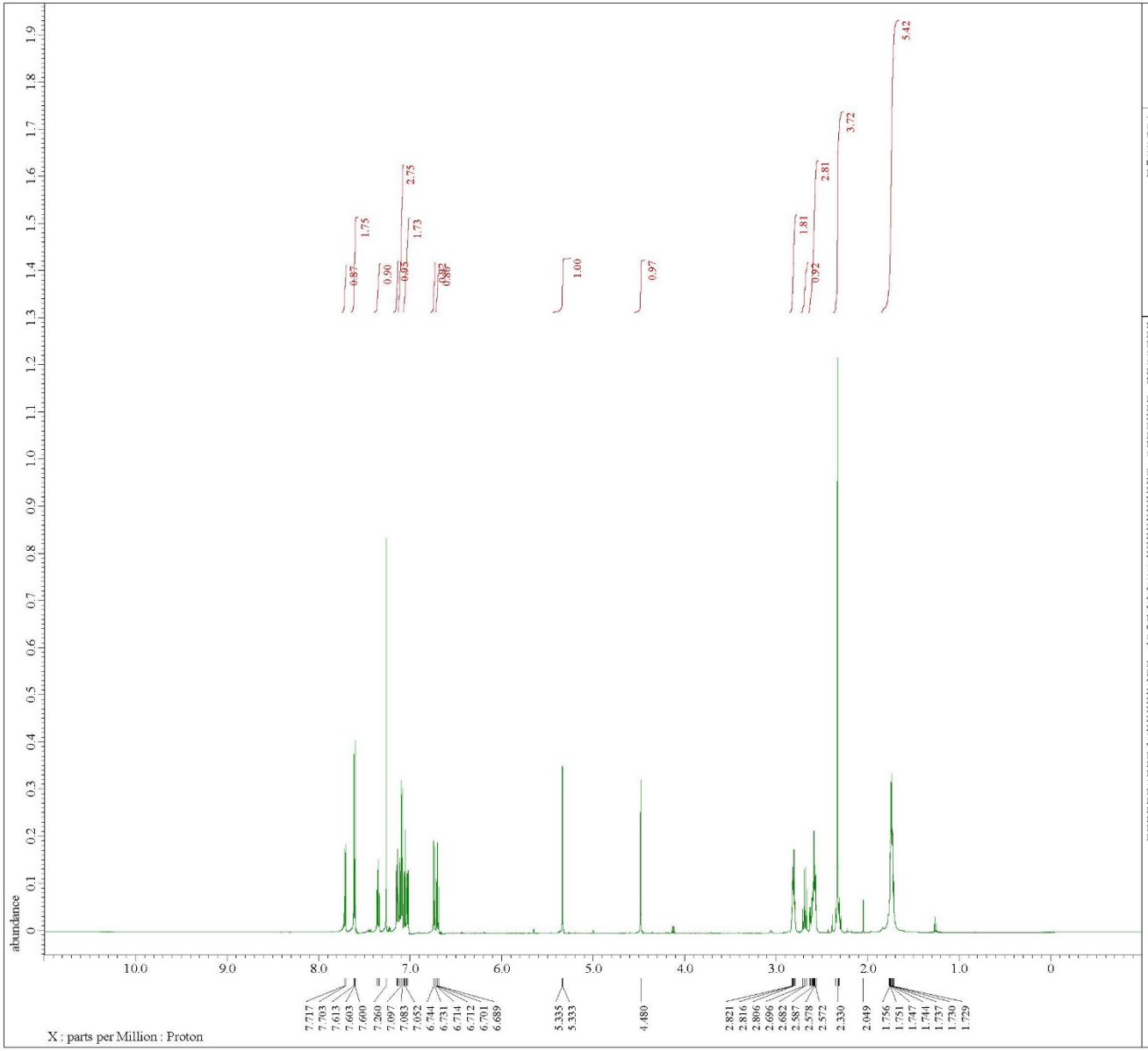
***trans*-4aqg**




```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

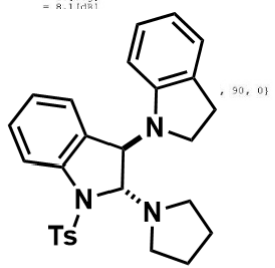
```
Filename                = KY-2-046-2-carbon-2
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = KY-2-046-2-carbon-2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 15-APR-2025 23:23:4
Revision_Time           = 16-APR-2025 08:35:3

Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (600
X_Acq_Duration          = 0.69206016[s]
X_Domain                = Carbon13
X_Freq                  = 150.91343039[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 1.44496109[Hz]
X_Sweep                 = 47.34848485[kHz]
X_Sweep_Clipped         = 37.87878788[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 15.0[us]
Clipped                 = FALSE
Scans
Total_Sca

Relaxatic
Recvr_Gai
Temp_Get
X_90_Widt
X_Acq_Tim                                  [s]
X_Angle
X_Atn
X_Pulse
Irr_Atn_D
Irr_Atn_D
Irr_Atn_D
Irr_Atn_N
Irr_Dec_R                                  [kHz]
Irr_Dec_R                                  8[ppm]
Irr_Dec_F                                  6[MHz]
Irr_Dec_M
Irr_Decou
Irr_Noe
Irr_Noise               = WALTZ
```


trans-4aqg

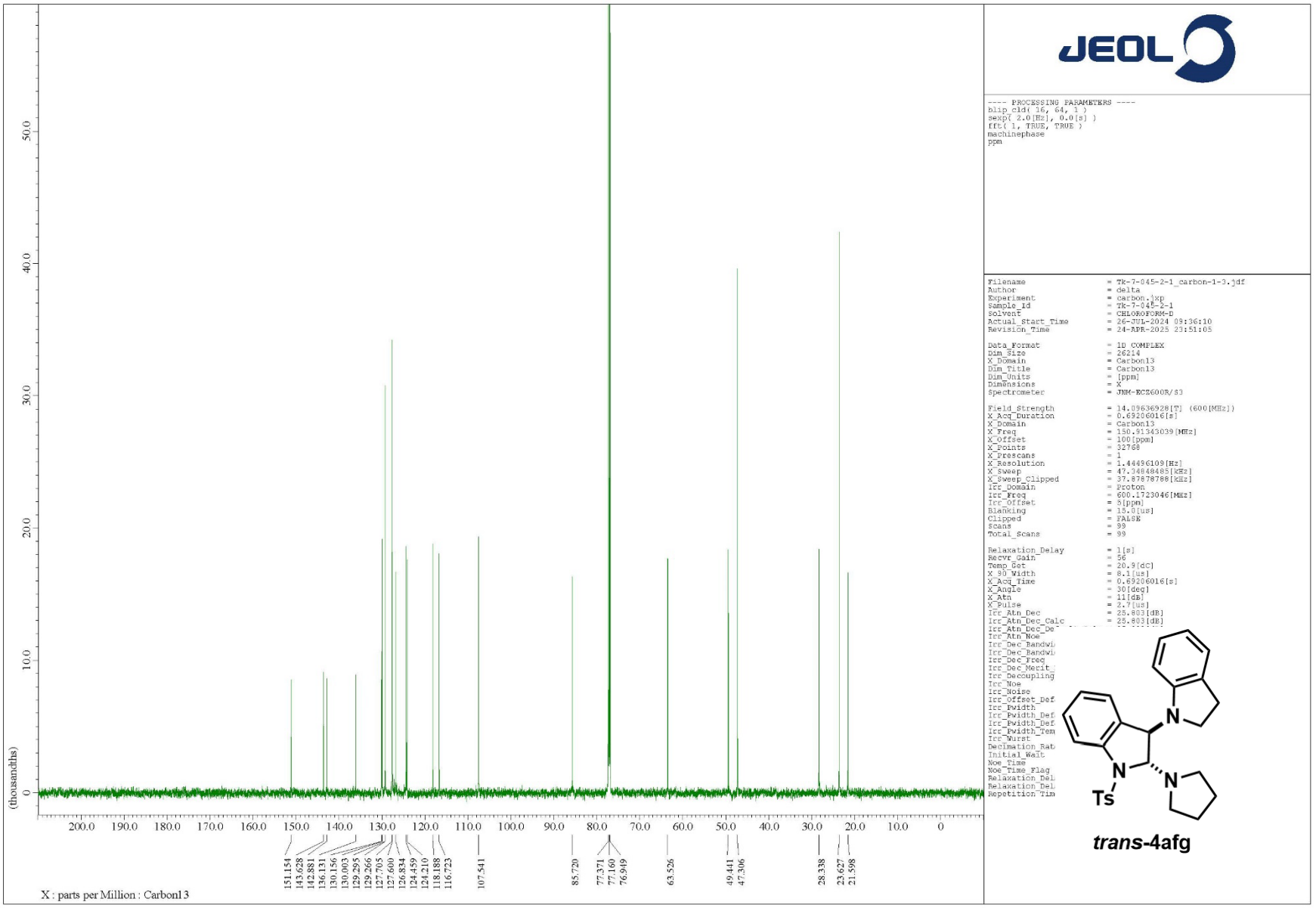


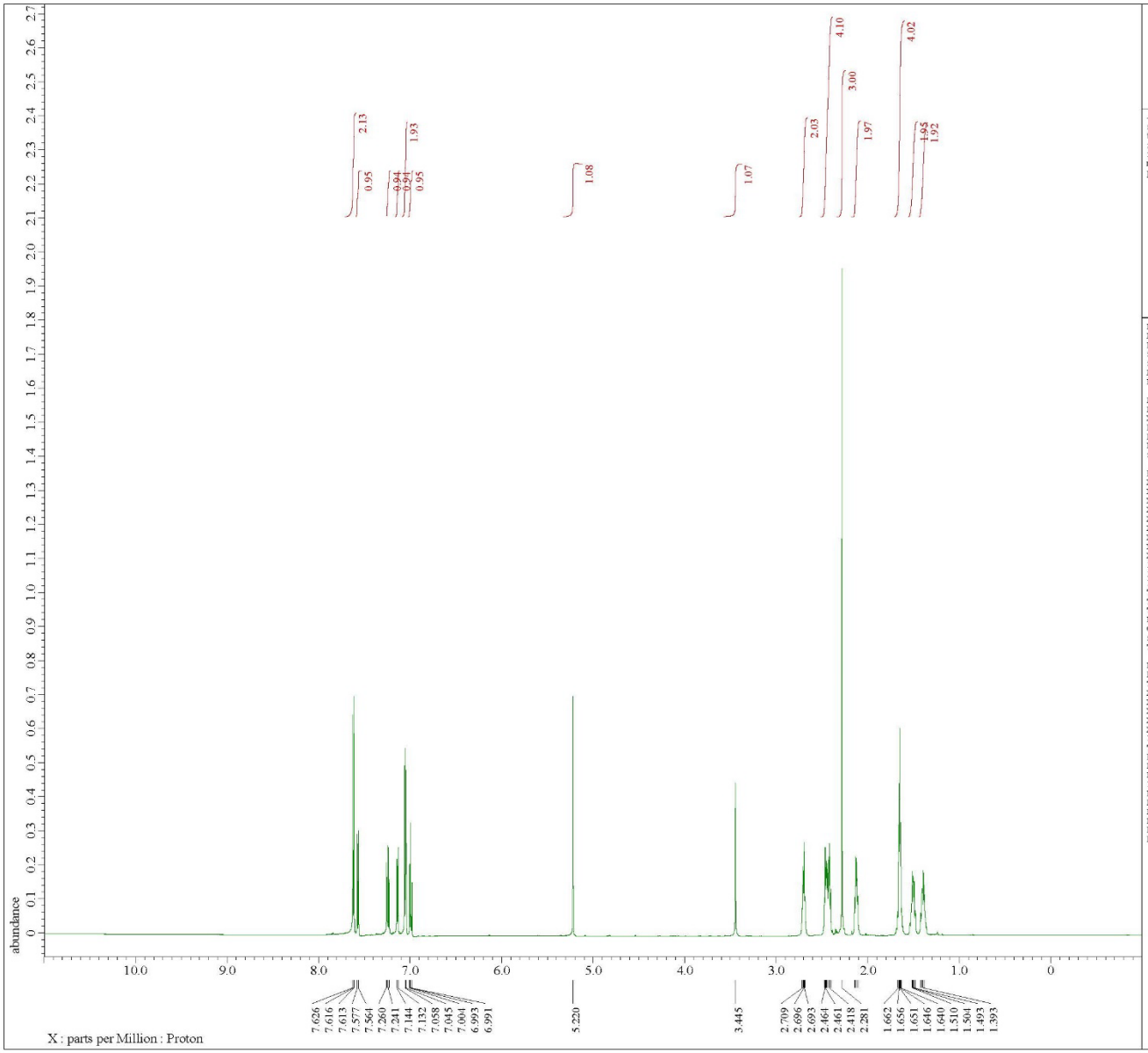
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm

Filename	= Tk-7-045-2-1_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-7-045-2-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-JUL-2024 09:35:28
Revision_Time	= 24-APR-2025 23:49:55
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 2.18365952[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45794685[Hz]
X_Sweep	= 15.0060024[kHz]
X_Sweep_Clipped	= 12.00480192[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 4
Total_Scans	= 4
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Set	= 20.9[dC]
X_90_Width	= 9.9[us]
X_Acq_Time	= 2.18365952[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	
Tri_Mode	
Tri_Mode	
Dante_Loop	
Dante_Presat	
Decimation_Rate	
Initial_Wait	
Phase	, 90, 0}
Presat_Time	
Presat_Time_Fla	
Relaxation_Dela	
Relaxation_Dela	
Repetition_Time	



***trans*-4afg**

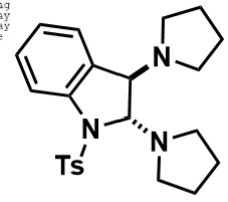

(thousandths)
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
151.154
143.628
142.881
136.131
130.156
130.003
129.295
129.266
127.705
127.600
126.834
124.459
124.210
118.188
116.723
107.541
85.720
77.371
77.160
76.949
63.526
49.441
47.306
28.338
23.627
21.598
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = Tk-7-045-2-1_carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Tk-7-045-2-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-JUL-2024 09:36:10
Revision_Time = 24-APR-2025 23:51:05
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 15.0[us]
Clipped = FALSE
Scans = 99
Total_Scans = 99
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 20.9[dC]
X_90_Width = 8.1[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 11[dB]
X_Pulse = 2.7[us]
Irr_Atn_Dec = 25.803[dB]
Irr_Atn_Dec_Calc = 25.803[dB]
Irr_Atn_Dec_De
Irr_Atn_Noe
Irr_Dec_Bandwi
Irr_Dec_Bandwi
Irr_Dec_Freq
Irr_Dec_Merit_
Irr_Decoupling
Irr_Noe
Irr_Noise
Irr_Offset_Def
Irr_Pwidth
Irr_Pwidth_Def
Irr_Pwidth_Def
Irr_Pwidth_Tem
Irr_Wurst
Decimation_Rat
Initial_Wait
Noe_Time
Noe_Time_Flag
Relaxation_Del
Relaxation_Del
Repetition_Tim
N
N
N
Ts
trans-4afg



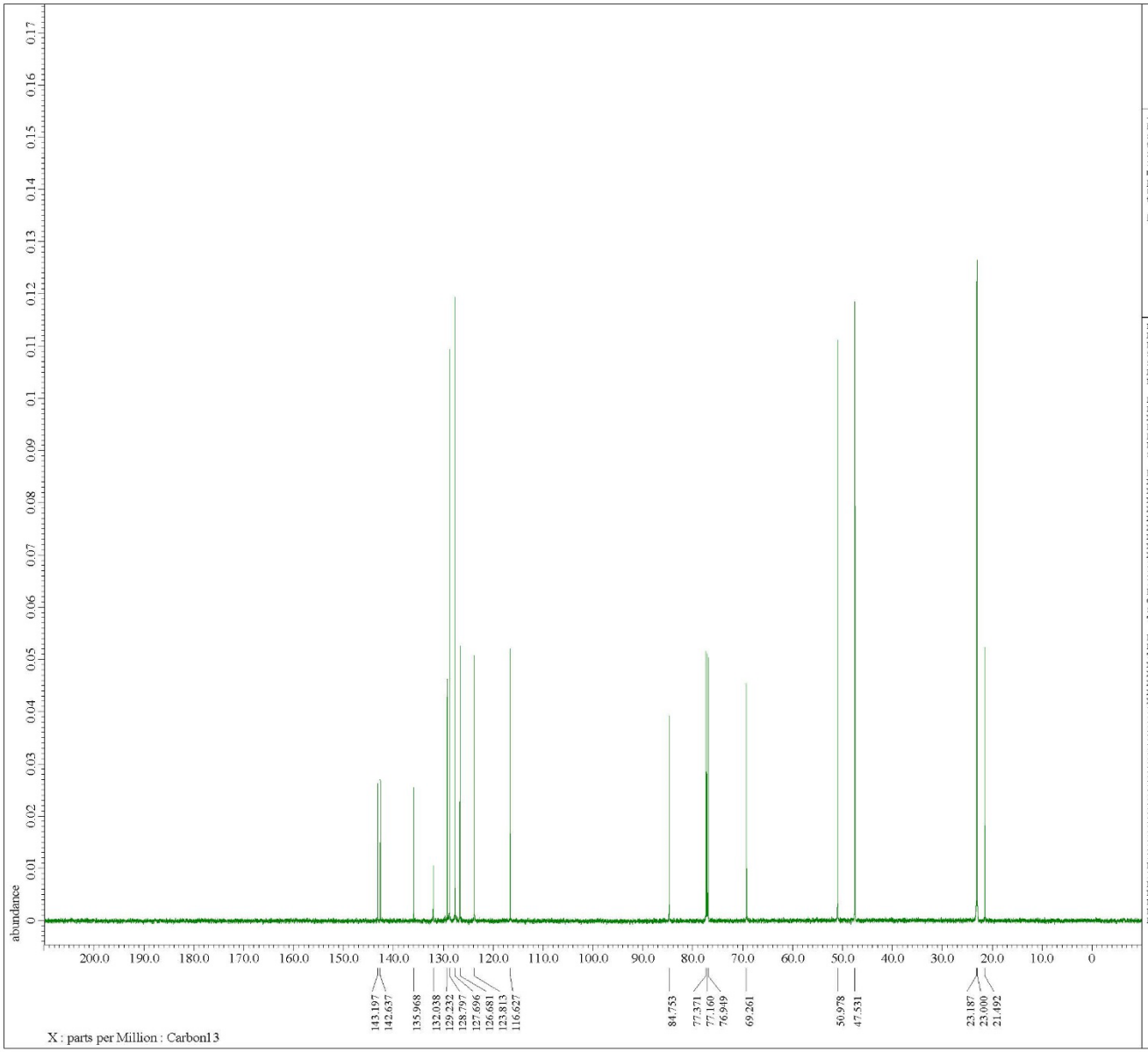
JEOL

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

Filename	= TK-7-029-1_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-7-025-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JUL-2024 17:12:39
Revision_Time	= 24-APR-2025 23:57:43
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 2.18365952[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45794685[Hz]
X_Sweep	= 15.0060024[kHz]
X_Sweep_Clipped	= 12.00480192[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 4
Total_Scans	= 4
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Set	= 20.9[dC]
X_90_Width	= 9.9[us]
X_Acq_Time	= 2.18365952[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 200
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	=
Presat_Time	
Presat_Time_Flag	
Relaxation_Delay	
Relaxation_Delay	
Repetition_Time	



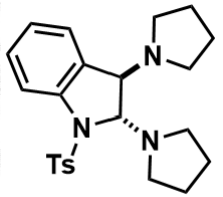
***trans*-4agg**



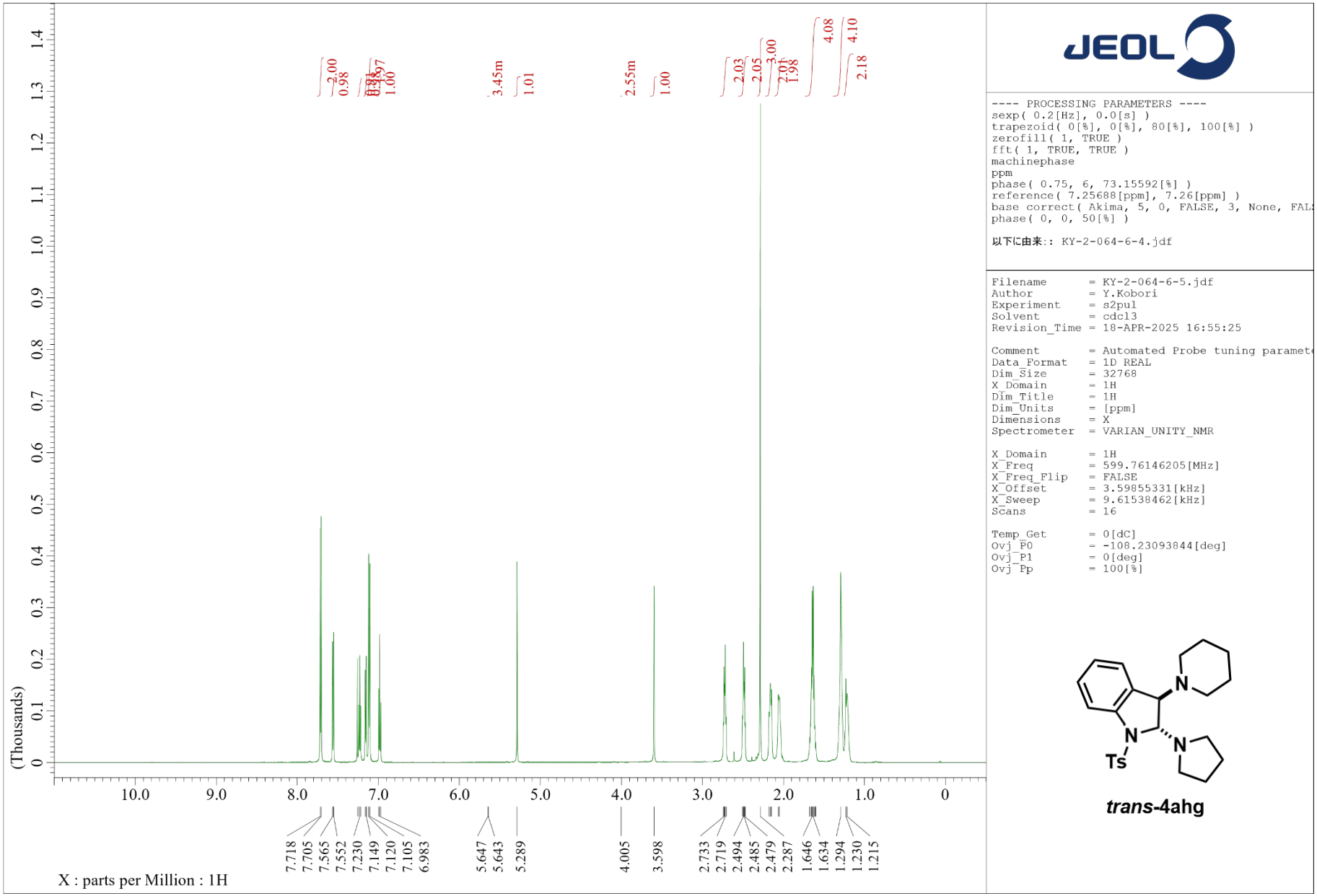
JEOL

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 1.44496[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.18812[ppm], 77.16[ppm] )
thresh( 5.9573[%], 1,  )

以下由来:: TK-7-029-1_carbon-1-1.jdf
```

Filename	= TK-7-029-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-7-029-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JUL-2024 17:47:04
Revision_Time	= 24-APR-2025 23:56:38
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91943039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.24848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15.0[us]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.5[dC]
X_90_Width	= 8.1[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 2.7[us]
Irr_Atn_Dec	= 25.803[dB]
Irr_Atn_Dec_Calc	= 25.803[dB]
Irr_Atn_Dec_Default_Calc	= 25.803[dB]
Irr_Atn_Noe	= 25.803[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwid	
Irr_Dec_Freq	
Irr_Dec_Merit_F	
Irr_Decoupling	
Irr_Noe	
Irr_Noise	
Irr_Offset_Defa	
Irr_Pwidth	
Irr_Pwidth_Defa	
Irr_Pwidth_Defa	
Irr_Pwidth_Temp	
Irr_Wurst	
Decimation_Rate	
Initial_Wait	
Noe_Time	
Noe_Time_Flag	
Relaxation_Dela	
Relaxation_Dela	
Repetition_Time	



***trans*-4agg**

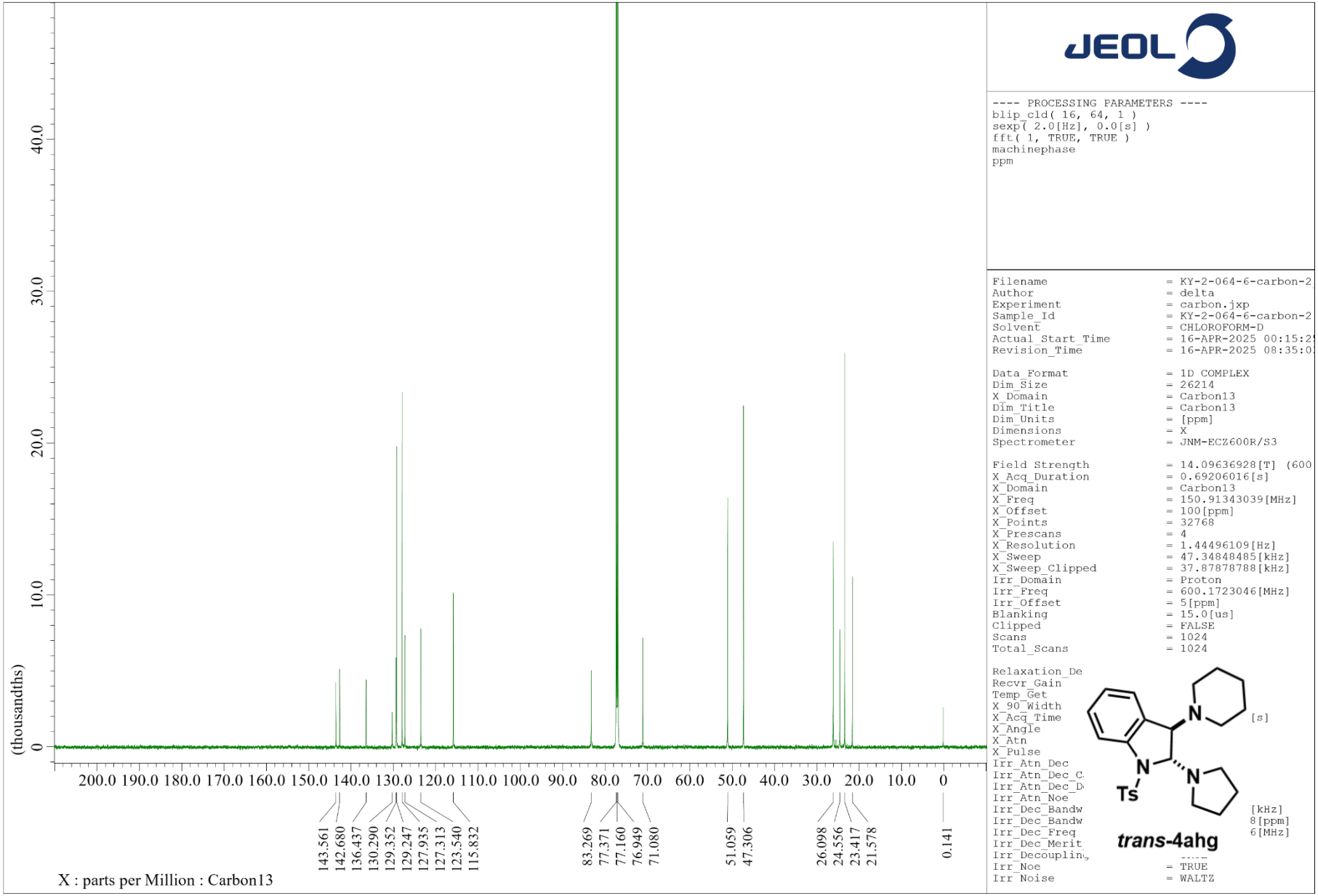


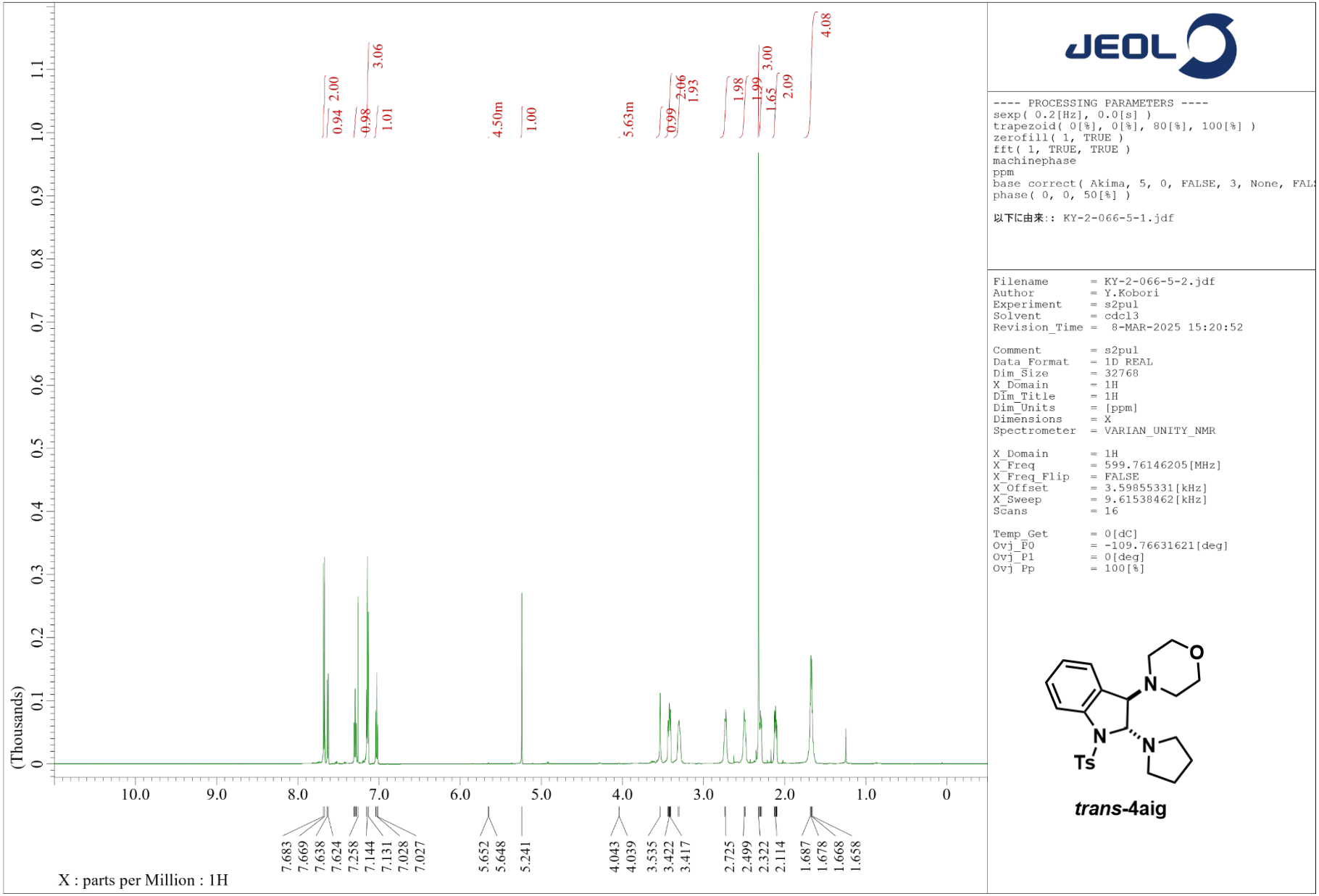
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 0.75, 6, 73.15592[%] )
reference( 7.25688[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-064-6-4.jdf
```

```
Filename       = KY-2-064-6-5.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 18-APR-2025 16:55:25

Comment        = Automated Probe tuning paramet
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 16

Temp_Get       = 0[dC]
Ovj_P0         = -108.23093844[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```


***trans*-4ahg**

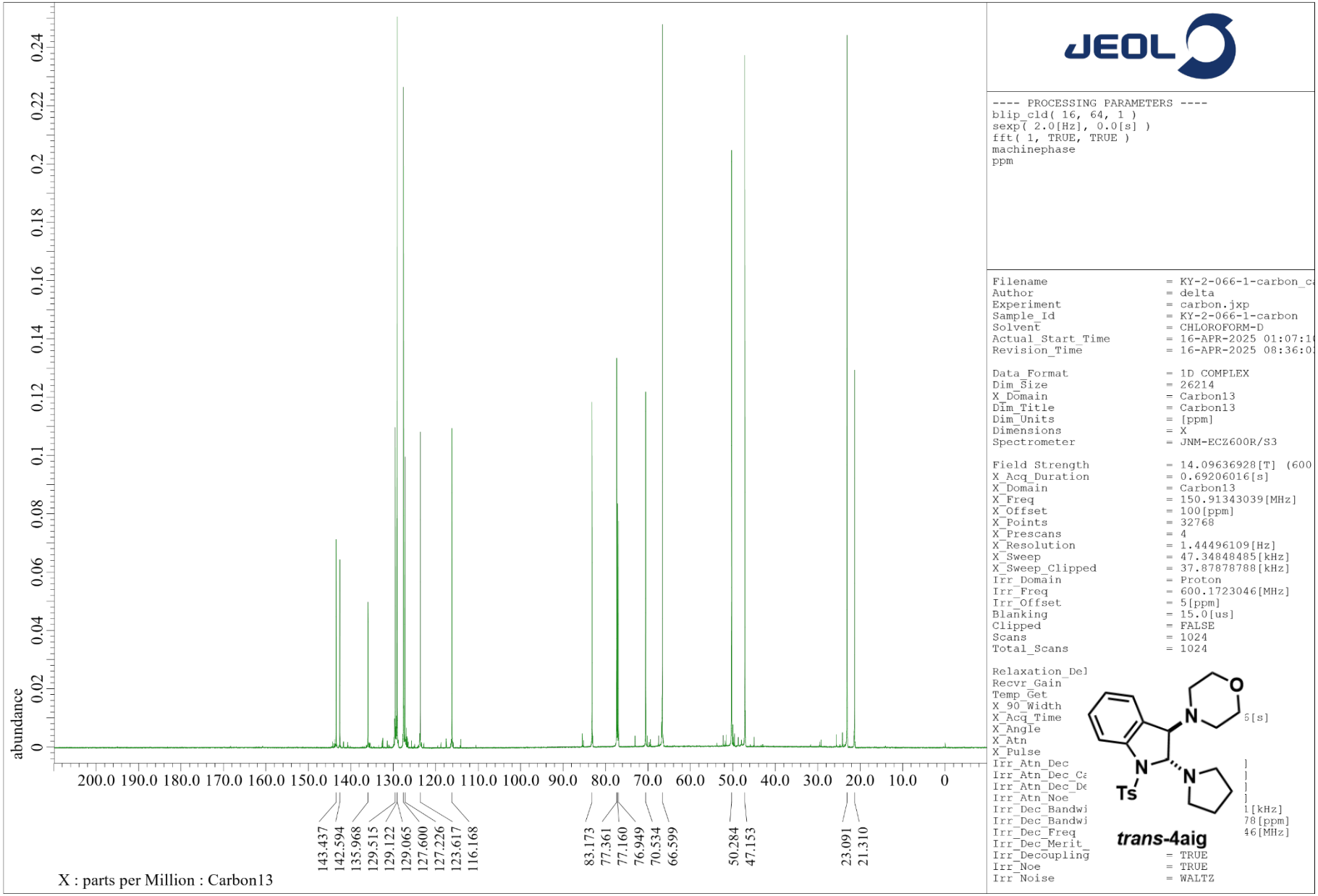

(thousandths)
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
143.561
142.680
136.437
130.290
129.352
129.247
127.935
127.313
123.540
115.832
83.269
77.371
77.160
76.949
71.080
51.059
47.306
26.098
24.556
23.417
21.578
0.141
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = KY-2-064-6-carbon-2
Author = delta
Experiment = carbon.jxp
Sample_Id = KY-2-064-6-carbon-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-APR-2025 00:15:2
Revision_Time = 16-APR-2025 08:35:0
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 15.0[us]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_De
Recvr_Gain
Temp_Get
X_90_Width
X_Acq_Time [s]
X_Angle
X_Atn
X_Pulse
Irr_Atn_Dec
Irr_Atn_Dec_C
Irr_Atn_Dec_D
Irr_Atn_Noe
Irr_Dec_Bandw [kHz]
Irr_Dec_Bandw 8[ppm]
Irr_Dec_Freq 6[MHz]
Irr_Dec_Merit
Irr_Decouplin
Irr_Noe = TRUE
Irr_Noise = WALTZ
N
N
N
Ts
trans-4ahg




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-066-5-1.jdf
```

```
Filename       = KY-2-066-5-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  =  8-MAR-2025 15:20:52

Comment        = s2pul
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 16

Temp_Get       = 0[dC]
Ovj_P0         = -109.76631621[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```


***trans*-4aig**

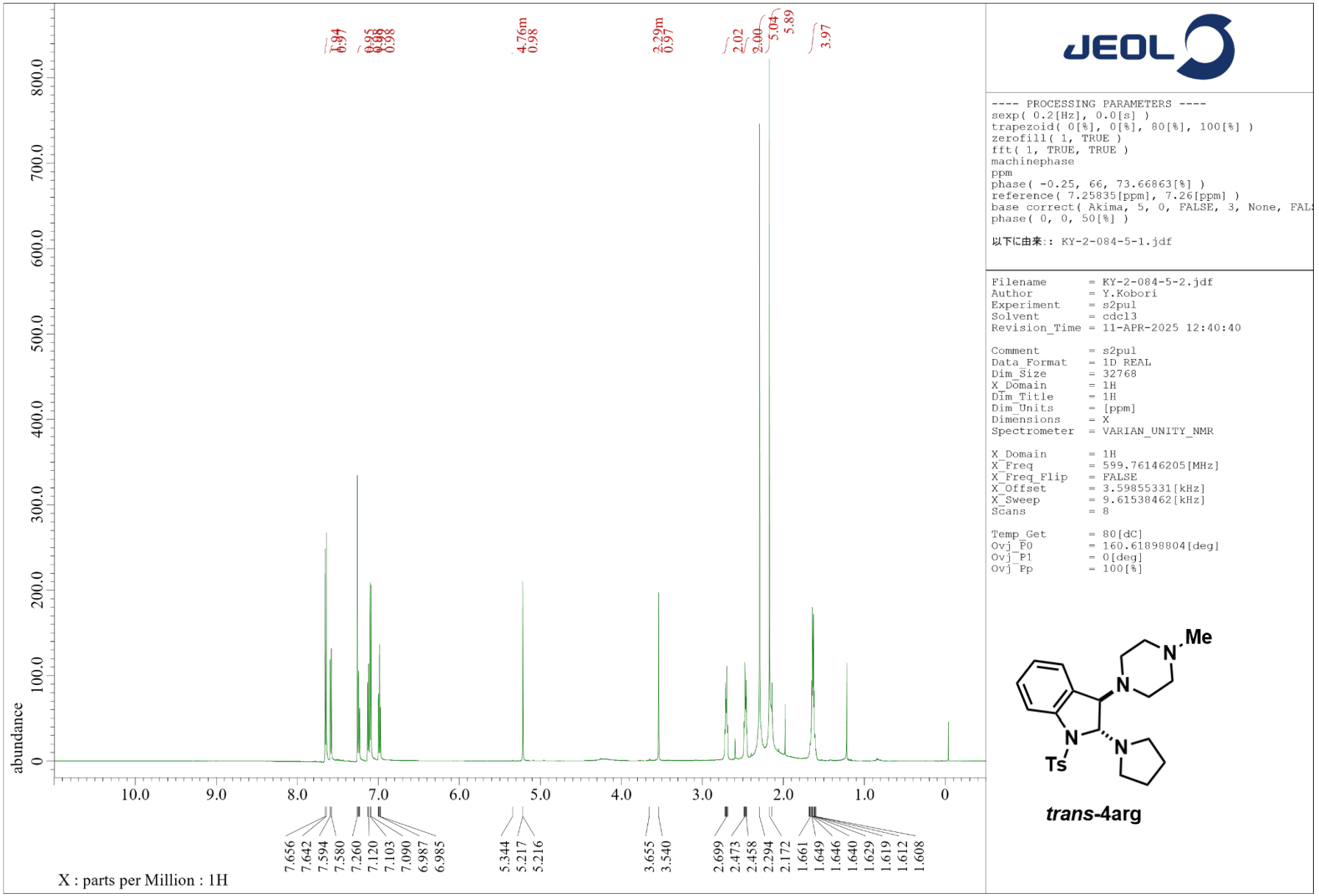


JEOL

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= KY-2-066-1-carbon_c
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-2-066-1-carbon
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-APR-2025 01:07:1
Revision_Time	= 16-APR-2025 08:36:0
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15.0[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Del	
Recvr_Gain	
Temp_Get	
X_90_Width	
X_Acq_Time	5[s]
X_Angle	
X_Atn	
X_Pulse	
Irr_Atn_Dec	]
Irr_Atn_Dec_Ca	]
Irr_Atn_Dec_De	]
Irr_Atn_Noe	]
Irr_Dec_Bandwi	1[kHz]
Irr_Dec_Bandwi	78[ppm]
Irr_Dec_Freq	46[MHz]
Irr_Dec_Merit_	
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ

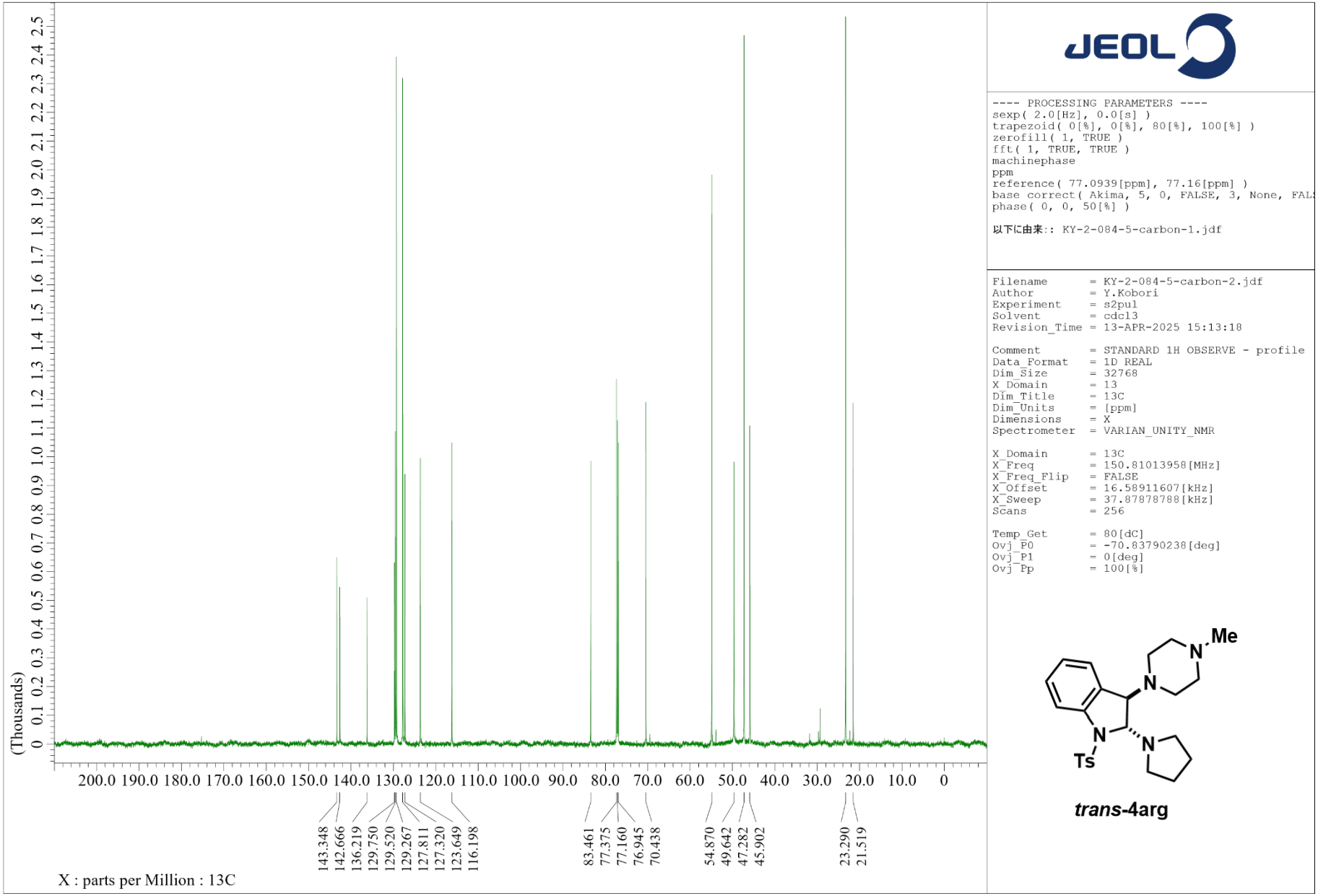
***trans*-4aig**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -0.25, 66, 73.66863[%] )
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-084-5-1.jdf
```

```
Filename       = KY-2-084-5-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 11-APR-2025 12:40:40

Comment        = s2pul
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = 160.61898804[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```

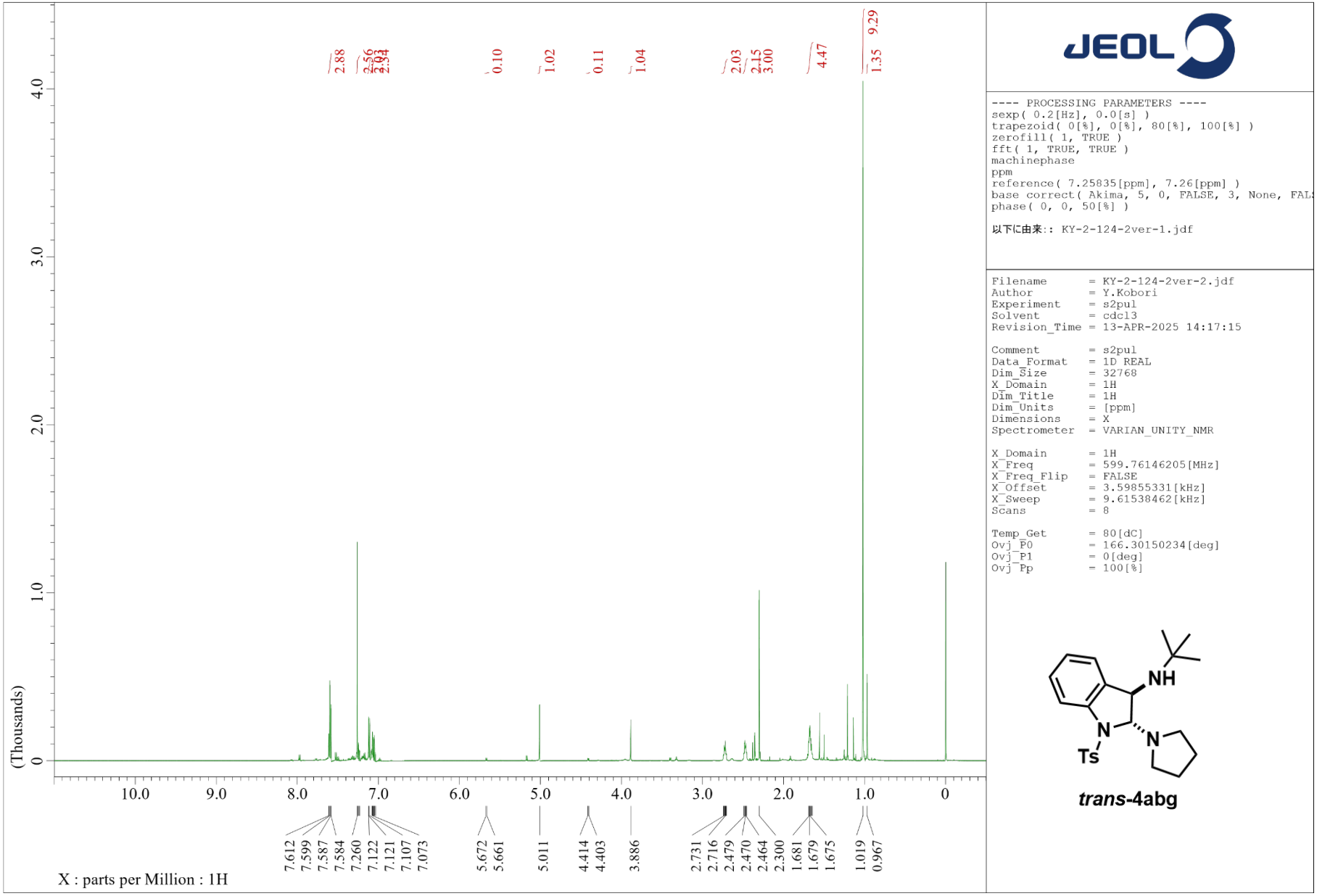

***trans*-4arg**




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.0939[ppm], 77.16[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-084-5-carbon-1.jdf
```

```
Filename       = KY-2-084-5-carbon-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 13-APR-2025 15:13:18

Comment        = STANDARD 1H OBSERVE - profile
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 13
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 13C
X_Freq         = 150.81013958[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 16.58911607[kHz]
X_Sweep        = 37.87878788[kHz]
Scans          = 256

Temp_Get       = 80[dC]
Ovj_P0         = -70.83790238[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```

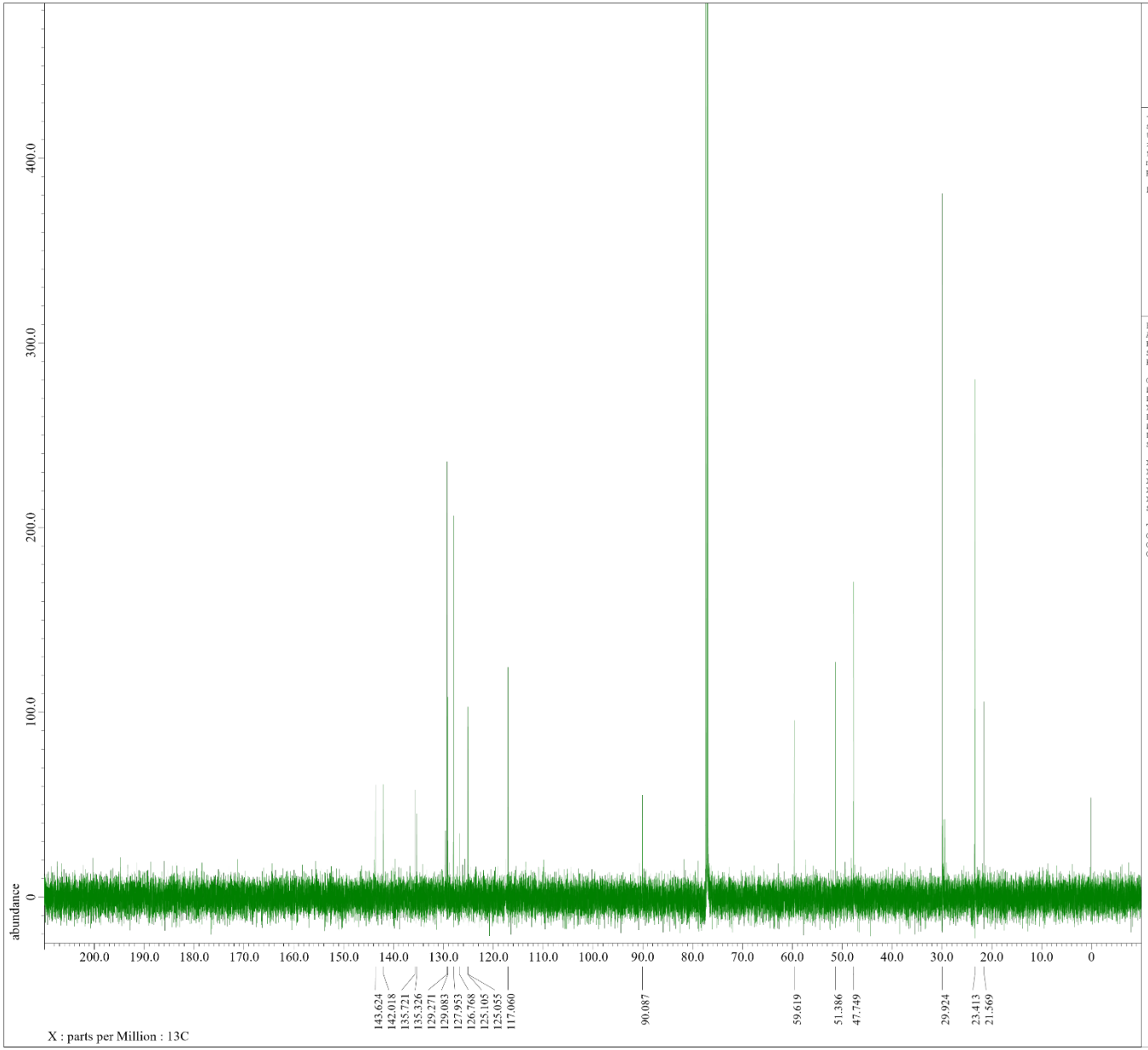

***trans*-4arg**




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.25835[ppm], 7.26[ppm] )
base correct( Akima, 5, 0, FALSE, 3, None, FAL
phase( 0, 0, 50[%] )

以下に由来:: KY-2-124-2ver-1.jdf
```

```
Filename       = KY-2-124-2ver-2.jdf
Author         = Y.Kobori
Experiment     = s2pul
Solvent        = cdcl3
Revision_Time  = 13-APR-2025 14:17:15

Comment        = s2pul
Data_Format    = 1D REAL
Dim_Size       = 32768
X_Domain       = 1H
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = VARIAN_UNITY_NMR

X_Domain       = 1H
X_Freq         = 599.76146205[MHz]
X_Freq_Flip    = FALSE
X_Offset       = 3.59855331[kHz]
X_Sweep        = 9.61538462[kHz]
Scans          = 8

Temp_Get       = 80[dC]
Ovj_P0         = 166.30150234[deg]
Ovj_P1         = 0[deg]
Ovj_Pp         = 100[%]
```

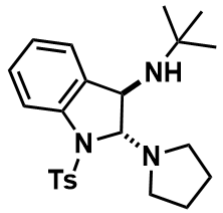

***trans*-4abg**



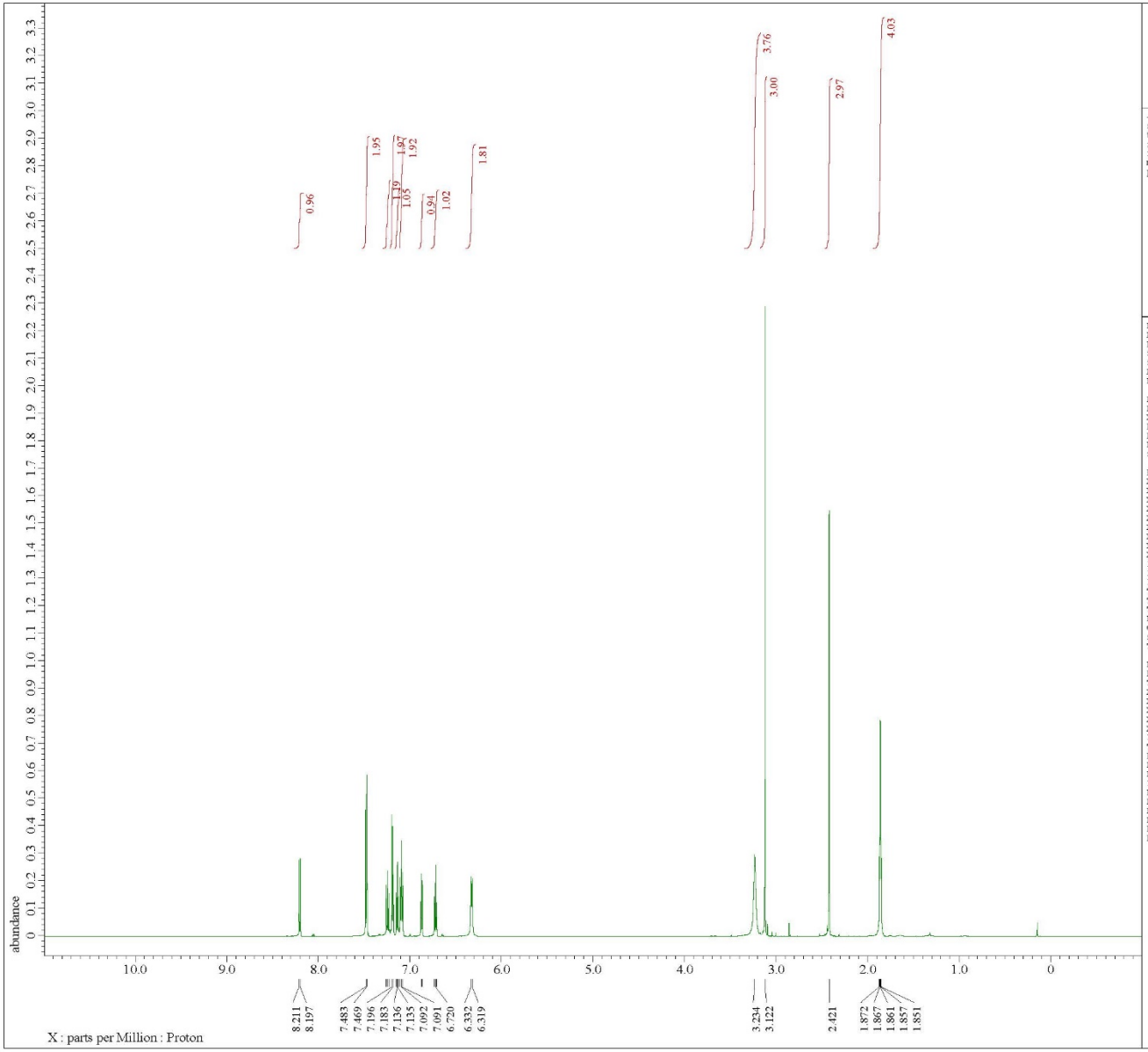
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.1[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: KY-2-124-2ver.2-carbon-2.jdf
```

```
Filename        = KY-2-124-2ver.2-carbon-3.jdf
Author          = 徳里慶祐
Experiment      = s2pul
Solvent         = cdcl3
Revision_Time   = 24-APR-2025 12:06:52

Comment         = s2pul
Data_Format     = 1D COMPLEX
Dim_Size        = 65536
X_Domain        = 13
DTm_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = VARIAN_UNITY_NMR

X_Domain        = 13C
X_Freq          = 150.81013958[MHz]
X_Freq_Flip     = FALSE
X_Offset        = 16.58911607[kHz]
X_Sweep         = 37.87878788[kHz]
Scans           = 256

Temp_Get        = 80[dC]
Ovj_T0          = 107.70112618[deg]
Ovj_P1          = 0[deg]
Ovj_Pp          = 100[%]
```

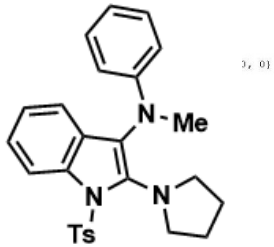


***trans*-4abg**

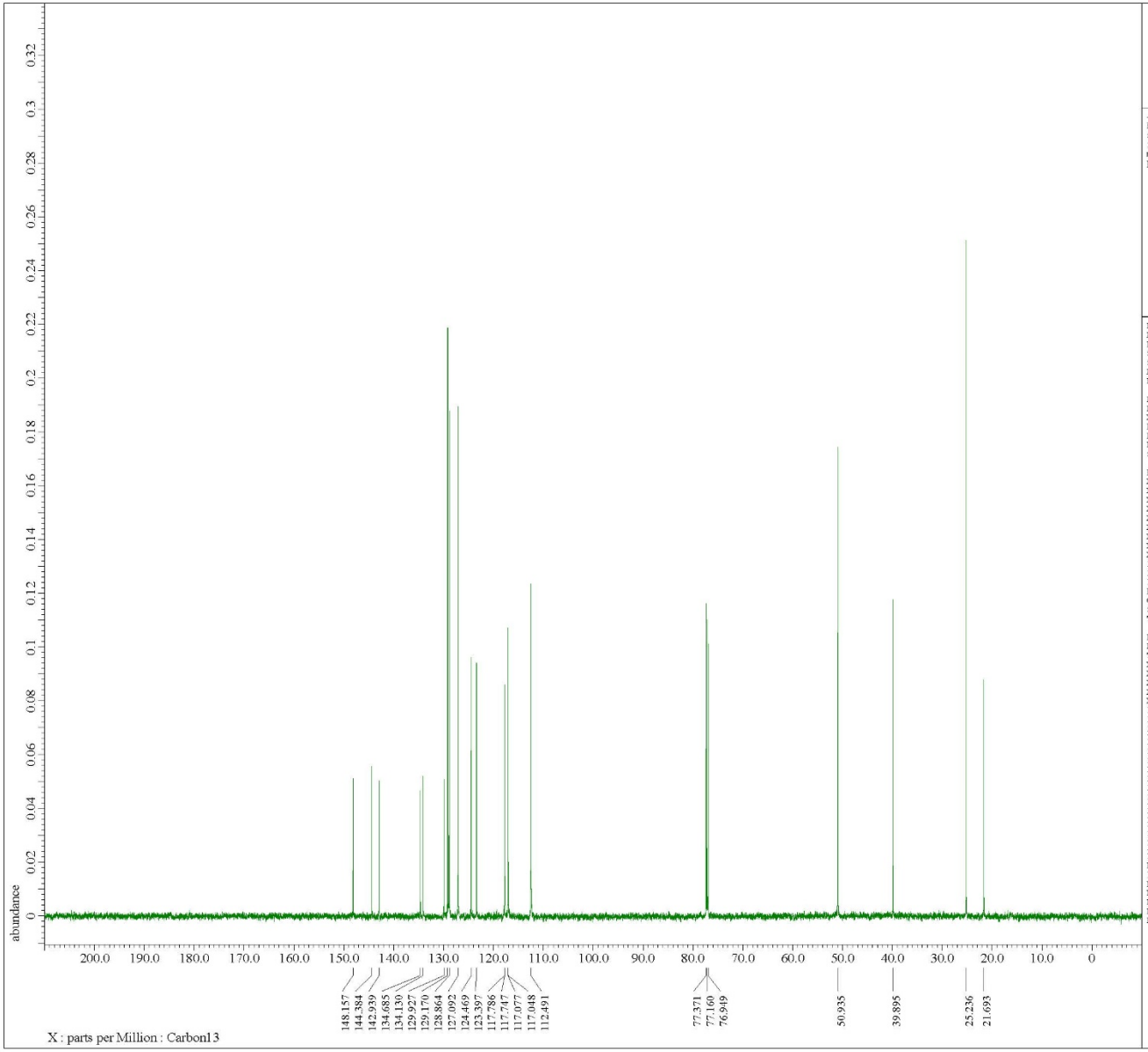


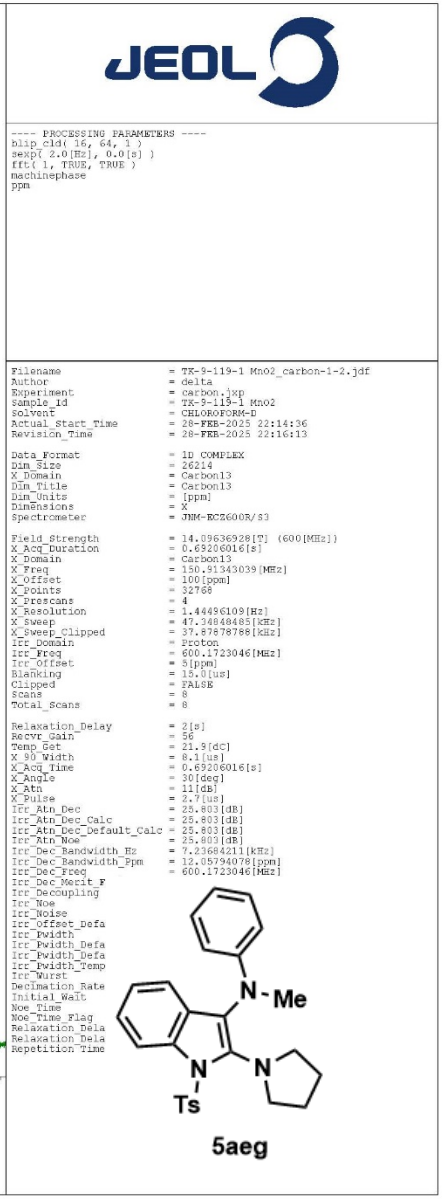

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= TK-9-119-1 MnO2_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_id	= TK-9-119-1 MnO2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-FEB-2025 22:12:09
Revision_Time	= 28-FEB-2025 23:00:43
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 2.90455552[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.34428676[Hz]
X_Sweep	= 11.28158845[kHz]
X_Sweep_Clipped	= 9.02527076[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 4
Total_Scans	= 4
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 22.1[dC]
X_90_width	= 10.5[us]
X_Acq_Time	= 2.90455552[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 5.25[us]
Irr_Mode	
Tri_Mode	
Dante_Loop	
Dante_Presat	
Decimation_Rat	
Initial_Wait	
Phase	3, 0)
Presat_Time	
Presat_Time_FL	
Relaxation_Del	
Relaxation_Del	
Repetition_Tim	



5aeg

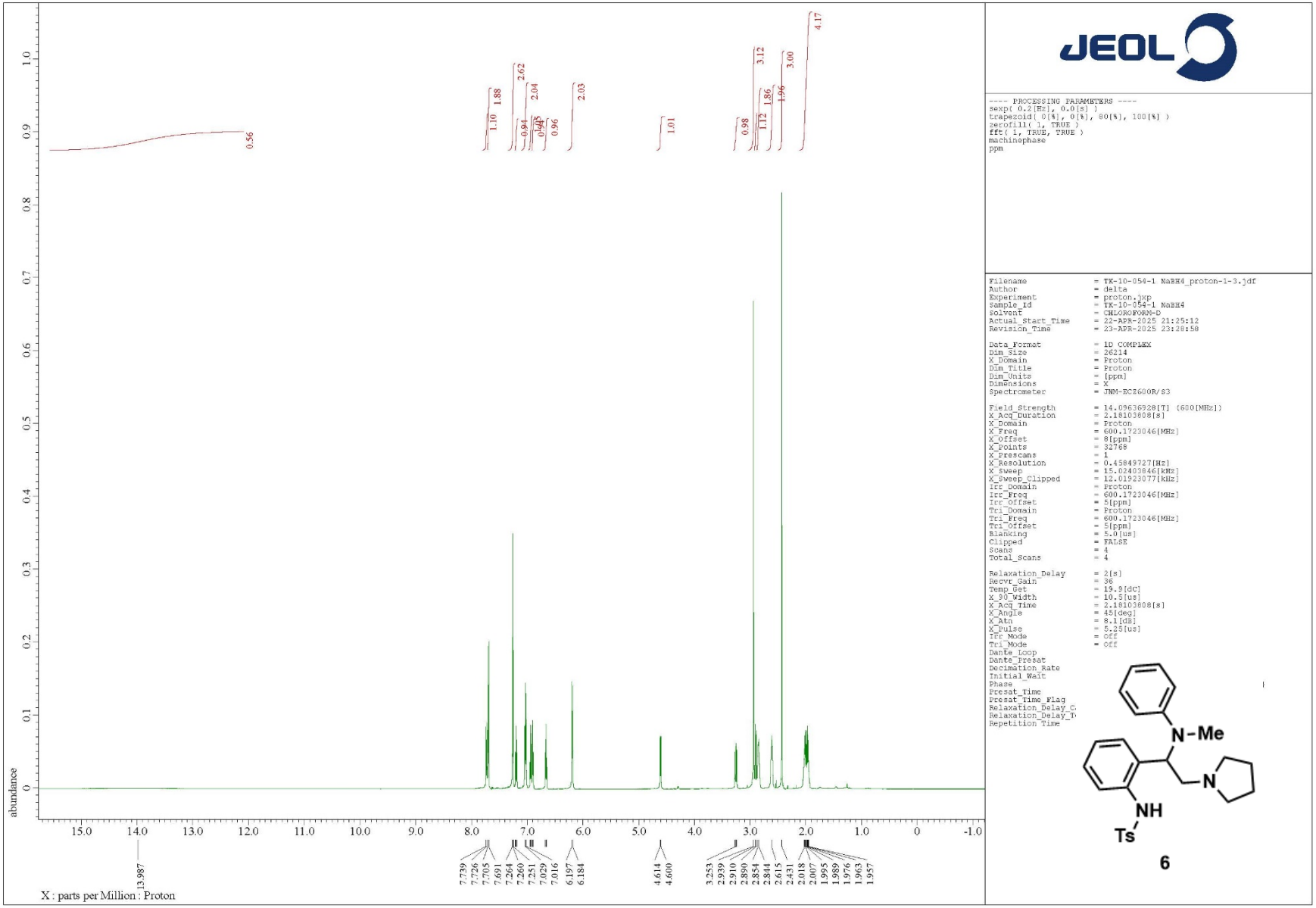




```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= TK-9-119-1 MnO2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-9-119-1 MnO2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-FEB-2025 22:14:36
Revision_Time	= 28-FEB-2025 22:16:13
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.81343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 21.9[dC]
X_90_Width	= 8.1[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 2.7[us]
Irr_Atn_Dec	= 25.803[dB]
Irr_Atn_Dec_Calc	= 25.803[dB]
Irr_Atn_Dec_Default_Calc	= 25.803[dB]
Irr_Atn_Noe	= 25.803[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_F	
Irr_DecCoupling	
Irr_Noe	
Irr_Noise	
Irr_Offset_Defa	
Irr_Pwidth	
Irr_Pwidth_Defa	
Irr_Pwidth_Defa	
Irr_Pwidth_Temp	
Irr_Wurst	
Decimation_Rate	
Initial_Wait	
Noe_Time	
Noe_Time_Flag	
Relaxation_Dela	
Relaxation_Dela	
Repetition_Time	

5aeg

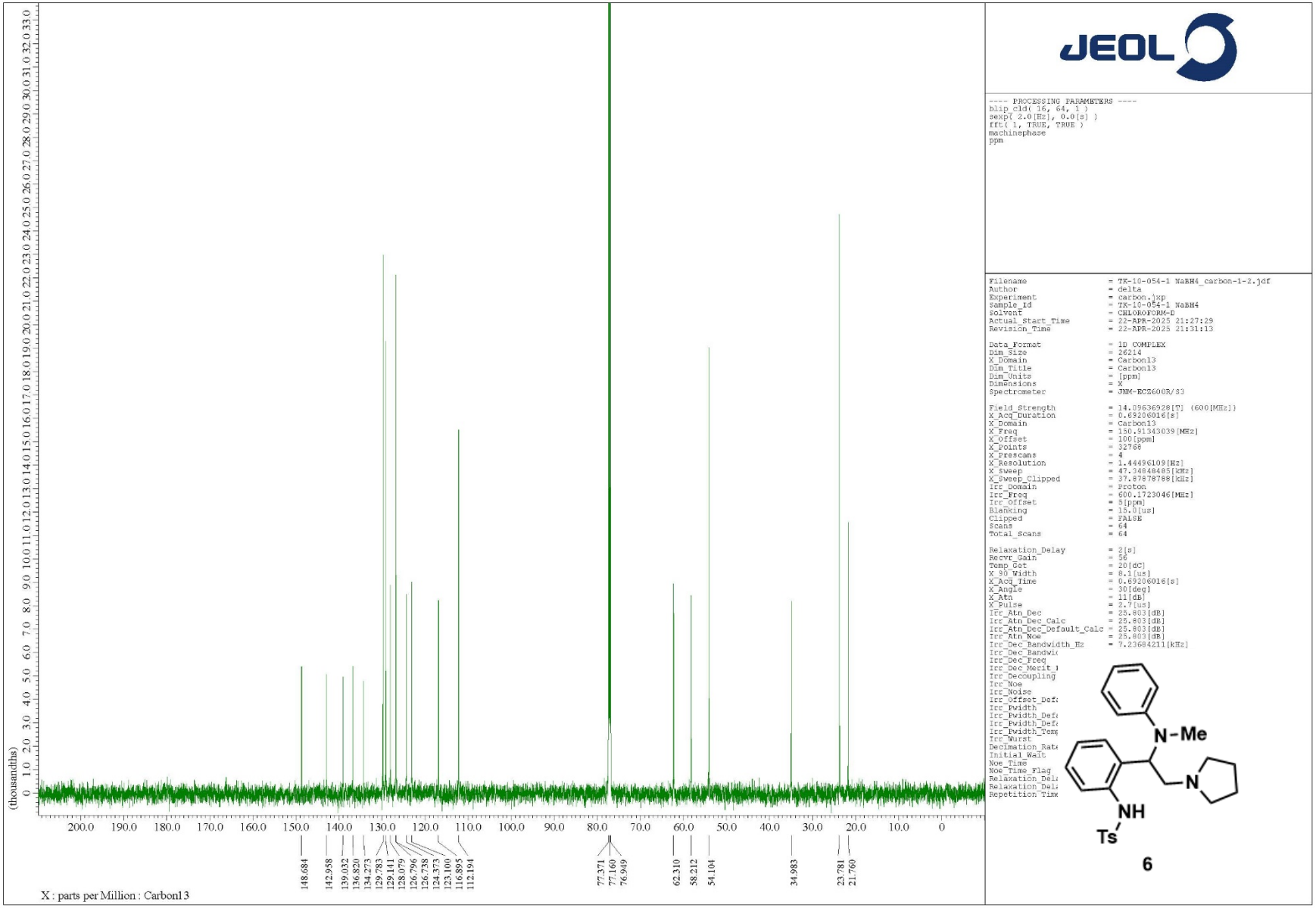


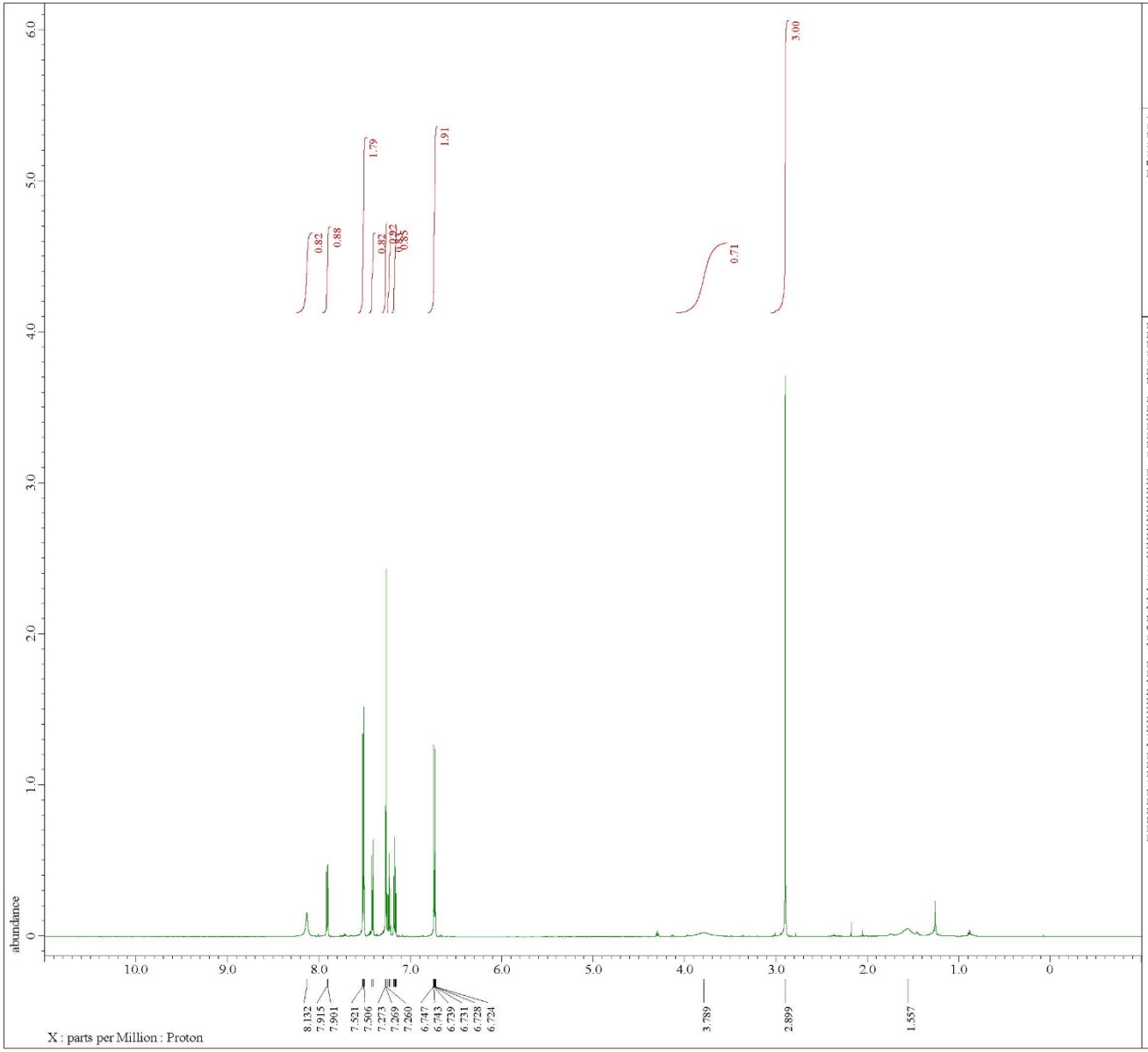
JEOL

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

Filename	= TK-10-054-1 NaBH4_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-10-054-1 NaBH4
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-APR-2025 21:25:12
Revision_Time	= 23-APR-2025 23:28:58
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 8[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.019230777[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 4
Total_Scans	= 4
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Set	= 19.9[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 5.25[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	
Dante_Presat	
Decimation_Rate	
Initial_Wait	
Phase	
Presat_Time	
Presat_Time_Flag	
Relaxation_Delay_C	
Relaxation_Delay_T	
Repetition_Time	

6

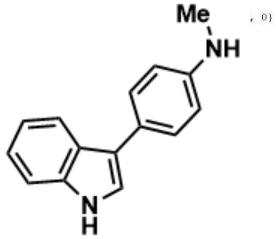

(thousandths)
X : parts per Million : Carbon13
148.684
142.958
139.032
136.820
134.273
129.783
129.141
128.079
126.796
126.738
124.373
123.100
116.895
112.194
77.371
77.160
76.949
62.310
58.212
54.104
34.983
23.781
21.760
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = TK-10-054-1 NaBH4_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-10-054-1 NaBH4
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-APR-2025 21:27:29
Revision_Time = 22-APR-2025 21:31:13
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.81343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 15.0[us]
Clipped = FALSE
Scans = 64
Total_Scans = 64
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20[dC]
X_90_Width = 8.1[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 11[dB]
X_Pulse = 2.7[us]
Irr_Atn_Dec = 25.803[dB]
Irr_Atn_Dec_Calc = 25.803[dB]
Irr_Atn_Dec_Default_Calc = 25.803[dB]
Irr_Atn_Noe = 25.803[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
N-Me
N
NH
Ts
6



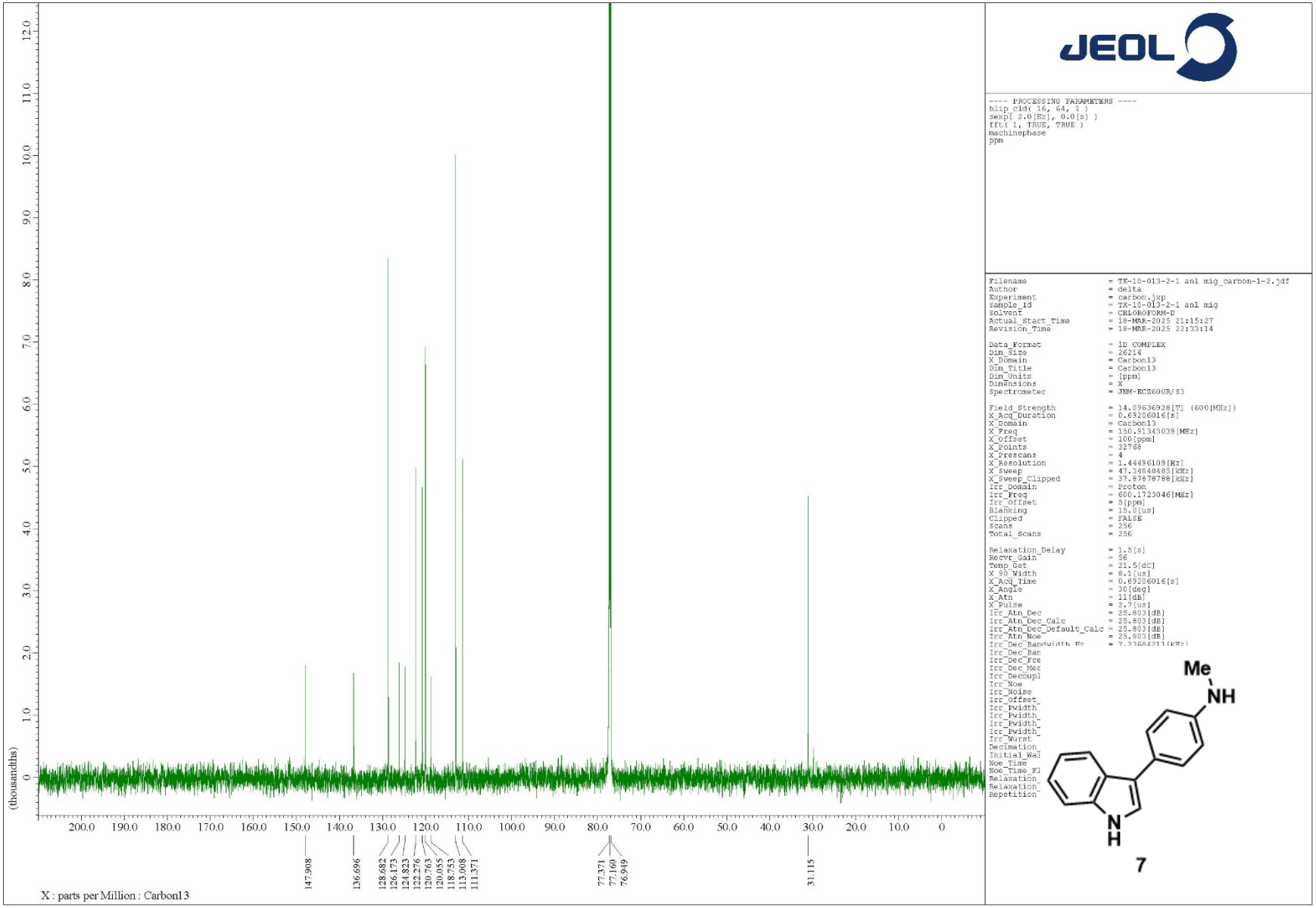
JEOL

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

Filename	= TK-10-013-2-1 anl mig_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-10-013-2-1 anl mig
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-MAR-2025 21:12:53
Revision_Time	= 18-MAR-2025 23:21:31
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 2.18103608[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Ifr_Domain	= Proton
Ifr_Freq	= 600.1723046[MHz]
Ifr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 21.4[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 2.18103608[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 5.25[us]
Ifr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 200
Dante_Presat	= [illegible]
Decimation_Rat	
Initial_Wait	
Phase	
Presat_Time	
Presat_Time_FL	
Relaxation_Del	
Relaxation_Del	
Repetition_Tim	



7



---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm

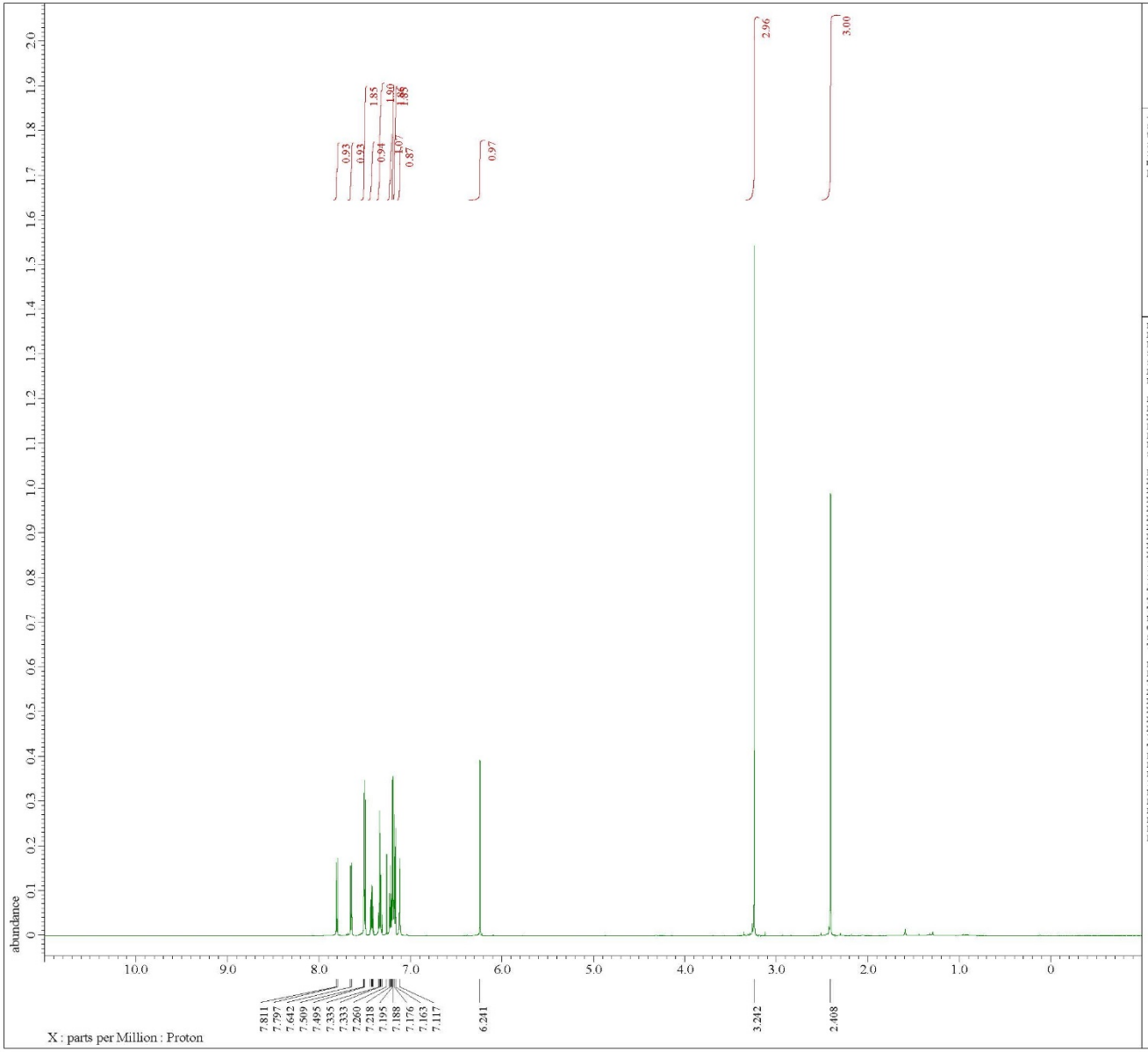
Filename = TX-10-013-2-1 anl mig_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TX-10-013-2-1 anl mig
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-MAR-2025 21:15:27
Revision_Time = 18-MAR-2025 22:33:14

Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.81343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 15.0[us]
Clipped = FALSE
Scans = 256
Total_Scans = 256

Relaxation_Delay = 1.5[s]
Recvr_Gain = 56
Temp_Get = 21.5[dC]
X_90_Width = 8.1[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 11[dB]
X_Pulse = 2.7[us]
Irr_Atn_Dec = 25.803[dB]
Irr_Atn_Dec_Calc = 25.803[dB]
Irr_Atn_Dec_Default_Calc = 25.803[dB]
Irr_Atn_Noe = 25.803[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Ban
Irr_Dec_Fre
Irr_Dec_Mer
Irr_DecCupl
Irr_Noe
Irr_Noise
Irr_Offset_
Irr_Pwidth_
Irr_Pwidth_
Irr_Pwidth_
Irr_Pwidth_
Irr_Wurst_
Decimation_
Initial_Wai
Noe_Time_
Noe_Time_Fl
Relaxation_
Relaxation_
Repetition_

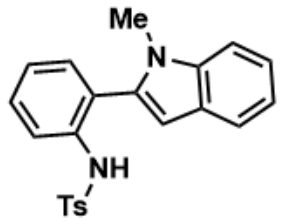
7



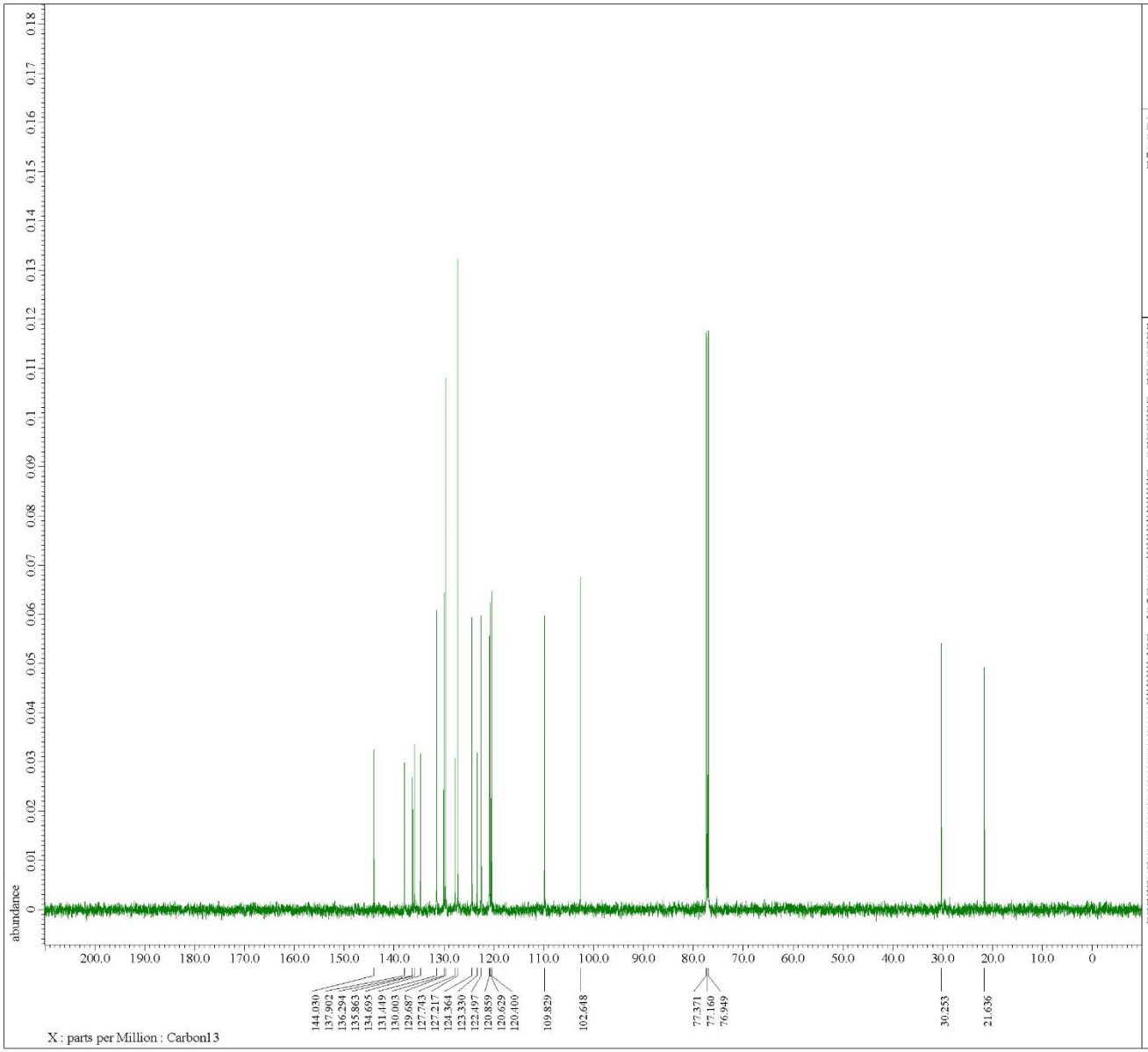
JEOL

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

Filename	= TK-9-117-1 RS_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-9-117-1 RS
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-FEB-2025 21:57:45
Revision_Time	= 27-FEB-2025 23:28:48
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 2.90455552[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.34428676[Hz]
X_Sweep	= 11.28158845[kHz]
X_Sweep_Clipped	= 9.02527076[kHz]
Ifr_Domain	= Proton
Ifr_Freq	= 600.1723046[MHz]
Ifr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 4
Total_Scans	= 4
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Set	= 20.8[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 2.90455552[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 5.25[us]
Ifr_Mode	= Off
Tri_Mode	
Dante_Loop	
Dante_Presat	
Decimation_Rat	
Initial_Wait	
Phase	
Presat_Time	
Presat_Time_Fl	
Relaxation_Del	
Relaxation_Del	
Repetition_Tim	



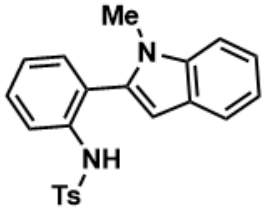
8



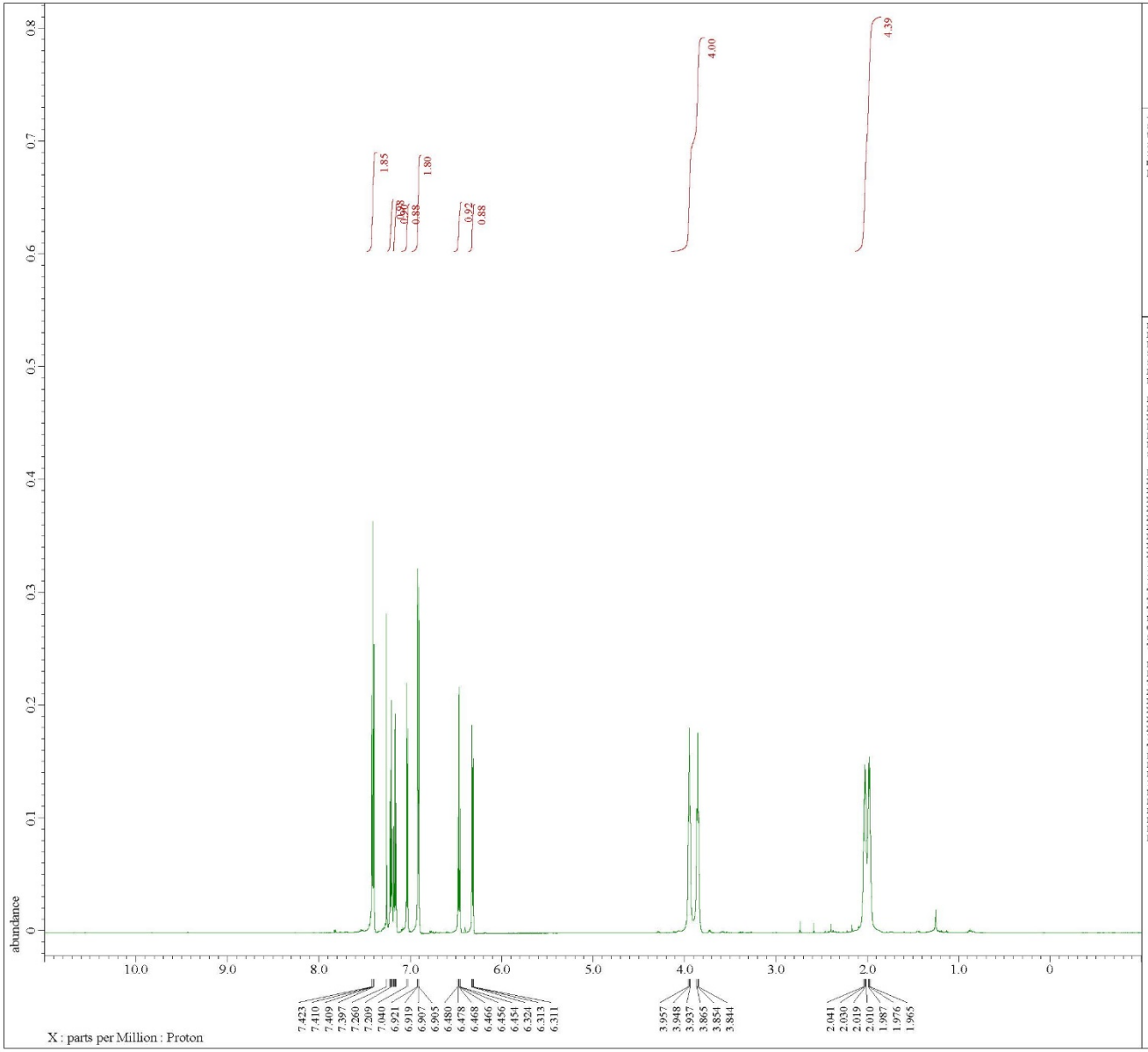
JEOL

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= TK-9-117-1 RS_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-9-117-1 RS
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-FEB-2025 22:00:08
Revision_Time	= 27-FEB-2025 22:01:39
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.24848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 21.2[dC]
X_90_Width	= 8.1[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 2.7[us]
Irr_Atn_Dec	= 25.803[dB]
Irr_Atn_Dec_Calc	= 25.803[dB]
Irr_Atn_Dec_Default_Calc	= 25.803[dB]
Irr_Atn_Noe	= 25.803[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	
Irr_Dec_Merit	
Irr_Decoupling	
Irr_Noe	
Irr_Noise	
Irr_Offset_Dec	
Irr_Pwidth	
Irr_Pwidth_Dec	
Irr_Pwidth_Dec	
Irr_Pwidth_Tes	
Irr_Wurst	
Decimation_Rat	
Initial_Wait	
Noe_Time	
Noe_Time_Flag	
Relaxation_Del	
Relaxation_Del	
Repetition_Tim	



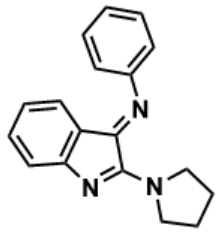
8



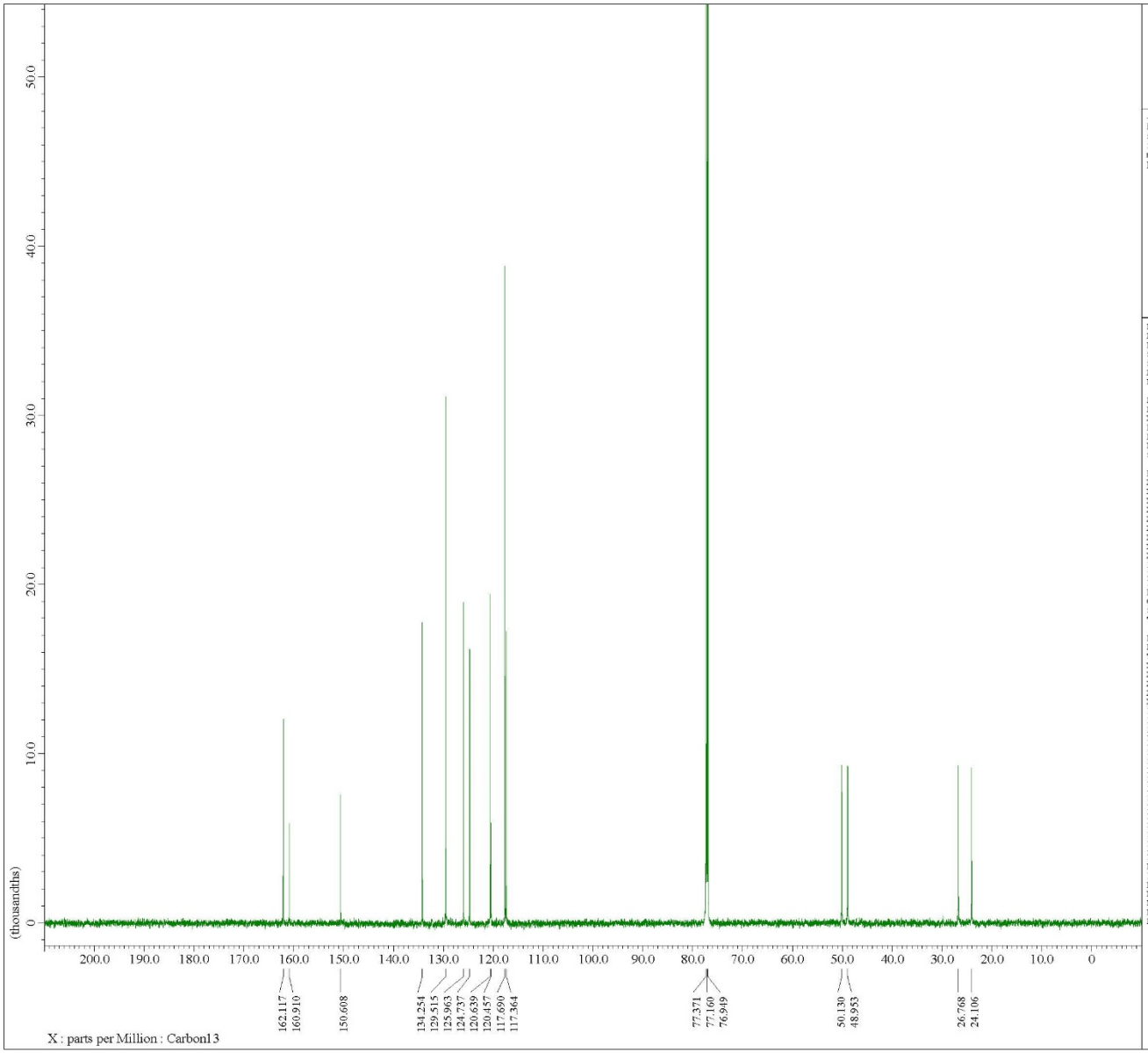
JEOL

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

Filename	= TK-10-003-5-3 MnO2 long_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-10-003-5-3 MnO2 long
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-MAR-2025 21:30:11
Revision_Time	= 18-MAR-2025 23:32:02
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 2.18103608[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Set	= 21.7[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 2.18103608[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 5.25[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 200
Dante_Presat	
Decimation_Rate	
Initial_Wait	
Phase	90, 0]
Presat_Time	
Presat_Time_Flag	
Relaxation_Delay	
Relaxation_Delay	
Repetition_Time	



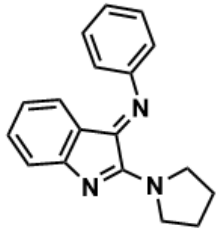
9



JEOL

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= TX-10-003-5-3 MnO2 long_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TX-10-003-5-3 MnO2 long
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-MAR-2025 21:32:40
Revision_Time	= 18-MAR-2025 22:35:56
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15.0[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 1.5[s]
Recvr_Gain	= 56
Temp_Get	= 21.7[dC]
X_90_Width	= 8.1[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 2.7[us]
Irr_Atn_Dec	= 25.803[dB]
Irr_Atn_Dec_Calc	= 25.803[dB]
Irr_Atn_Dec_Default_Calc	= 25.803[dB]
Irr_Atn_Noe	= 25.803[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	
Irr_Dec_Merit_Fact	
Irr_Decoupling	
Irr_Noe	
Irr_Noise	
Irr_Offset_Default	
Irr_Pwidth	
Irr_Pwidth_Default	
Irr_Pwidth_Default	
Irr_Pwidth_Temp1	
Irr_Wurst	
Decimation_Rate	
Initial_Wait	
Noe_Time	
Noe_Time_Flag	
Relaxation_Delay_C	
Relaxation_Delay_T	
Repetition_Time	



9