Indoline Hemiaminals: A Platform for Accessing Anthranilic Acid Derivatives through Oxidative Deformylation

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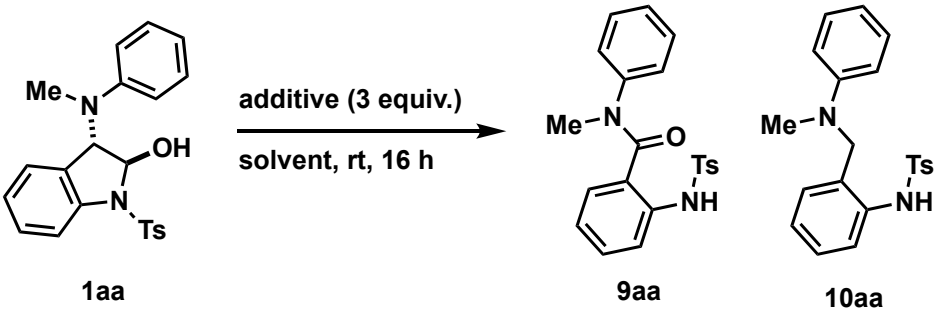
Supporting Information

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. 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.

Table S1. Optimization of reaction conditions[a] [1]



1aa **9aa** **10aa**

Entry	Additive	solvent	Yield (%) of **9aa**[b]	Yield (%) of **10aa**[b]
1	***tert*-BuOK**	**THF**	**81**	**3**
2	*tert*-BuOK	toluene	75	1
3	*tert*-BuOK	MeCN	66	5
4	*tert*-BuOK	MeOH	65	0
5	*tert*-BuOK	CH_2Cl_2	71	0
6	*tert*-BuOK	DMF	76	4
7	***tert*-BuOK**	**DMSO**	**81**	**3**
8[c]	*tert*-BuOK	DMSO	61	3
9[d]	*tert*-BuOK	DMSO	72	2
10[e]	*tert*-BuOK	DMSO	49	0
11[f]	*tert*-BuOK	DMSO	1	0
12[g]	*tert*-BuOK	DMSO	trace	0
13[h]	*tert*-BuOK	DMSO	80	0
14	*tert*-BuONa	DMSO	79	0
15	*tert*-BuOLi	DMSO	60	0
16	NaOH	DMSO	80	0
17	KOH	DMSO	77	0
18	K_2CO_3	DMSO	24	4
19	$CsCO_3$	DMSO	74	0
20	Et_3N	CH_2Cl_2	trace	-
21	none	DMSO	0	0

[a] Reaction condition: 1aa (1.0 mmol) and additive in solvent (5 mL, 0.2 M) under Air. [b] Isolated yield. [c] Using 5 equiv. of *tert*-BuOK. [d] Using 2 equiv. of *tert*-BuOK. [e] Using 1 equiv. of *tert*-BuOK. [f] Under argon. [g] The reaction was performed in DMSO with FTP cycling under argon. [h] Under O_2 (1 atm).

Synthesis of *N*-protected indoles S1

The *N*-potected indoles **S1** as *N*-tosylindoles (**S1a**, **S1e–S1k**), *N*-benzenesulfonylindole (**S1b**), *N*-(4-methoxybenzenesulfonyl)indole (**S1c**), *N*-mesylindole (**S1d**) and *N*-(4-phenylbenzenesulfonyl)indole (**S1l**) 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]

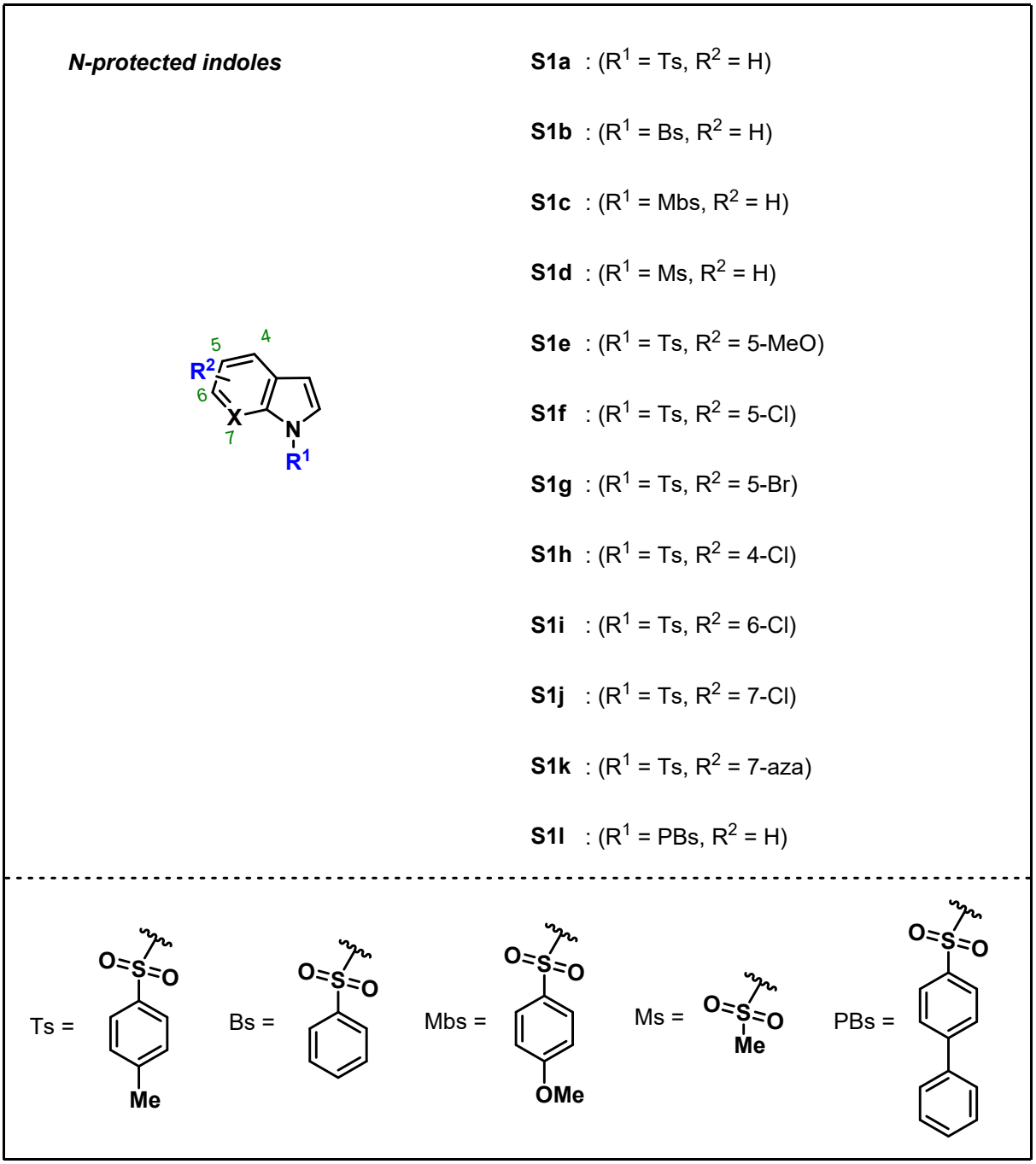
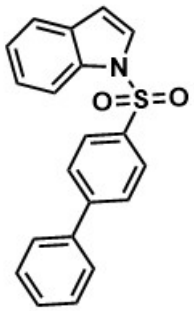


Figure S1.



S1l

1-([1,1'-Biphenyl]-4-ylsulfonyl)-1*H*-indole (S1l).[2] To a solution of indole (1.17 g, 10 mmol) and tetrabutylammonium bromide (161 mg, 0.05 equiv., 0.5 mmol) in toluene (10 mL, 0.1 M) were added NaOH (4.00 g, 10equiv., 0.10 mol) and H_2O (8.0 mL). The solution was stirred at room temperature for 15 minutes, biphenyl sulfonyl chloride (2.78 g, 1.1 equiv., 11 mmol) was added to the solution. After the solution was stirred further 12 h, H_2O (50 mL) was added to the mixture. The whole was extracted with AcOEt (3 x 50 mL). The combined organic layer was washed with brine (50 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt (5/1 v/v) to give **S1l**.

White solid (2.07 g, 62% yield; mp 105–108 °C). IR (KBr) ν: 3392, 3369, 1361, 1166, 761 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 4.2 Hz, 1H), 7.55 (d, J =7.8 Hz, 1H), 7.50 (d, J = 7.2 Hz, 2H), 7.43 (dd, J = 7.2, 7.2 Hz, 2H), 7.39 (dd, J = 7.8, 7.8 Hz, 1H), 7.34 (ddd, J = 7.8, 7.8, 0.6 Hz, 1H), 7.24 (ddd, J = 7.8, 7.8, 0.6 Hz, 1H), 6.69 (dd, J = 3.6, 0.6 Hz, 1H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 146.9, 139.0, 136.8, 135.0, 130.9, 129.2, 128.8, 128.0, 127.45, 127.45, 126.5, 124.8, 123.5, 121.6, 113.7, 109.4. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{20}H_{15}NO_2SNa$ 356.0721; Found 356.0720.

Synthesis of *trans*-2-hydroxyindoline-3-trirthylammonium bromide (HITAB) S2

The *trans*-2-hydroxyindoline-3-triethylammonium bromides (HITAB) **S2** 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 (S2a[3a], S2b, S2g, S2i[3b], S2c, S2d[3c], S2e, S2f[3d]).

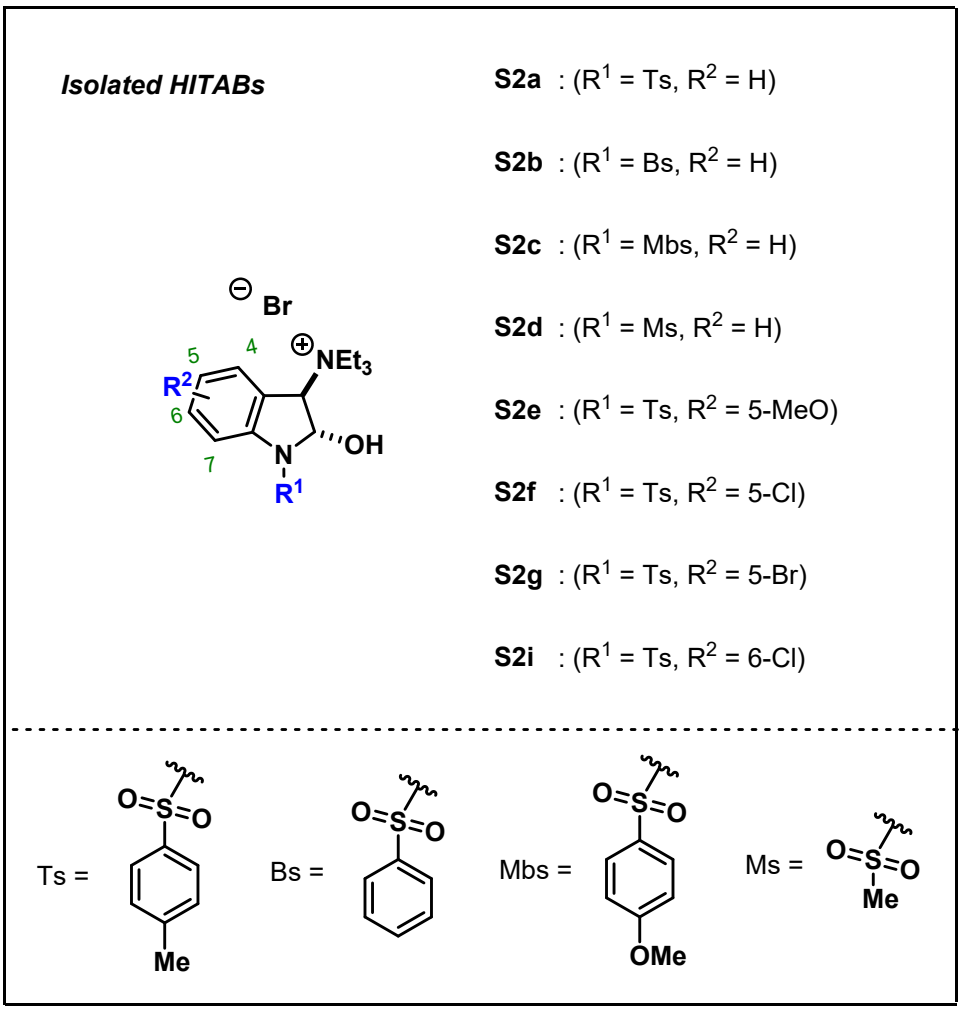


Figure S2.

Synthesis of indoline hemiaminals 8

The indoline hemiaminals **8** were prepared by reported method.[1b, 3, 4] All reagents were weighed and handled in air at 80 °C. Analytical data are in accordance with the literature values.(8aa [3a], 8ba–8ga, 8ia, 8ka [3c], 8ab, 8ac, 8ae, 8ah–8al, 8ar, 8as [1b], 8ag [4])

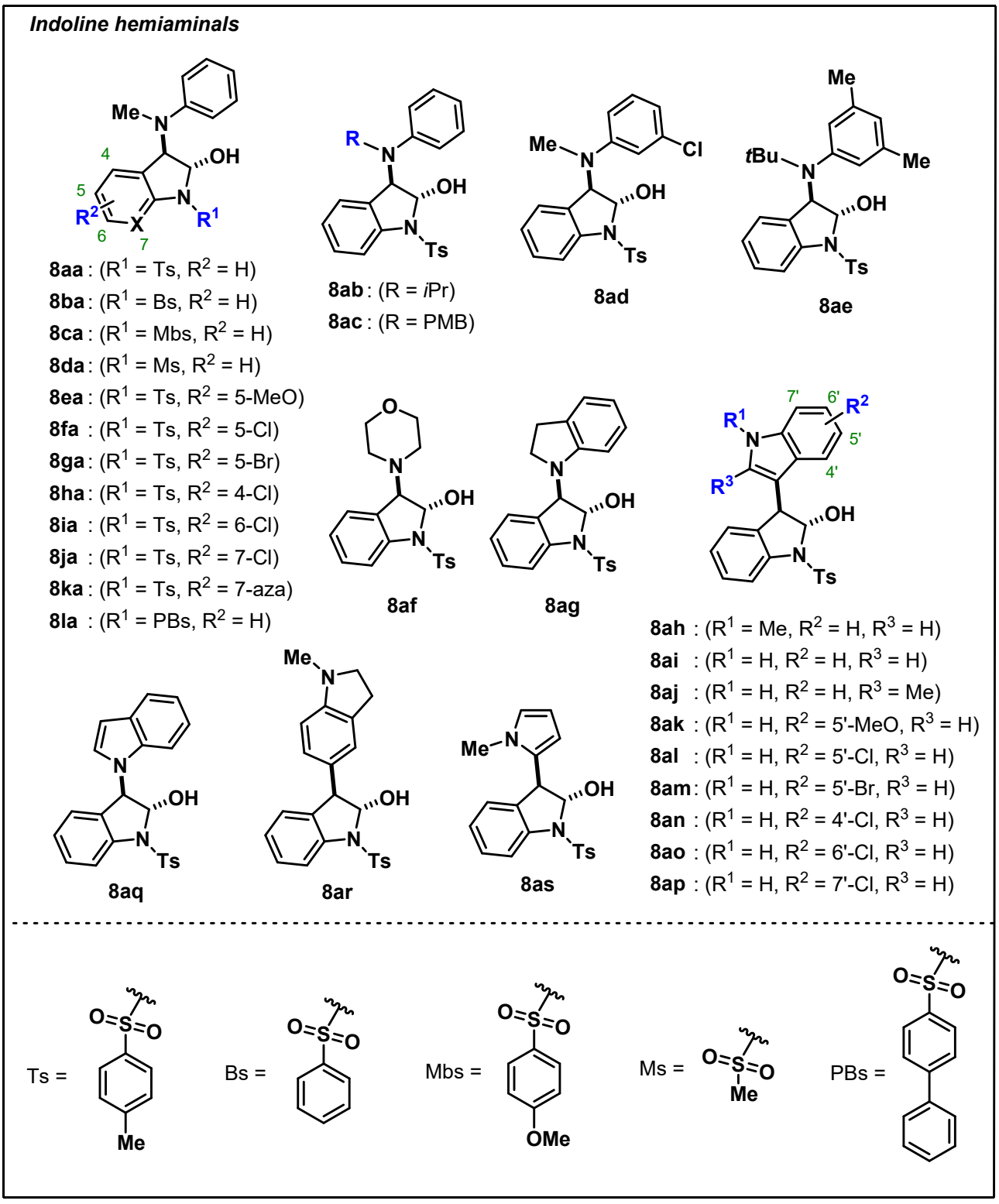
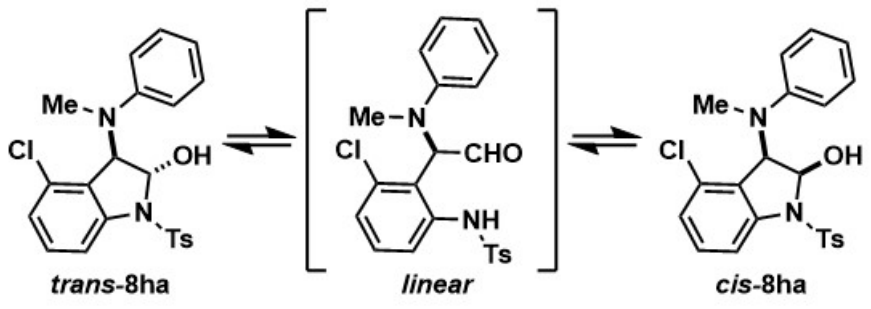


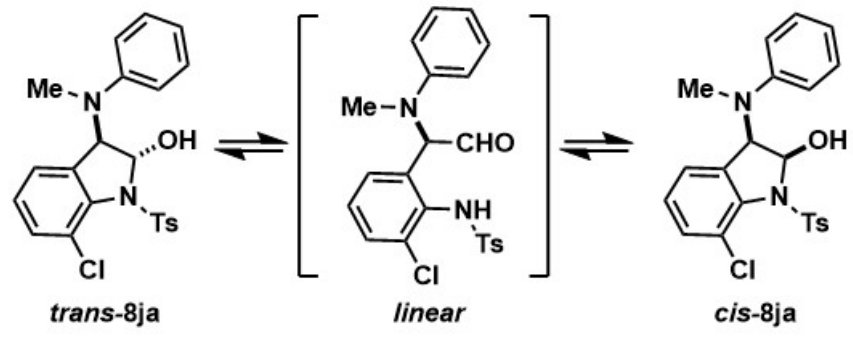
Figure S3.



(*trans*:*cis* = 95:5)

(*rac*)-*trans*-4-Chloro-3-(methyl(phenyl)amino)-1-tosylindolin-2-ol (8ha).[4] To a solution of **S1h** (1.22 mg, 2 equiv., 10 mmol) and H_2O (1.8 mL, 20 equiv., 0.1 mol) in acetone (50 mL, 0.2 M) was added NBS (1.98 g, 2.2 equiv., 11 mmol). The mixture was stirred at room temperature for 15 h. Then Et_3N (1.54 mL, 2.2 equiv., 11 mmol) was added to the mixture and stirred further 1 h. The mixture was concentrated *in vacuo*. The residue was dissolved in AcOEt (50 mL, 0.1 M) and added *N*-methylaniline (0.54 mL, 5.0 mmol) and Et_3N (1.39 mL, 2.0 equiv., 10 mmol). The mixture was stirred at 80 °C in oil bath for 23 hours. After the whole was cooled to room temperature, H_2O (50 mL) was added to the mixture. The whole was extracted with AcOEt (3 x 50 mL). The combined organic layer was washed with brine (50 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt (3/1 v/v) to give **8ha**.

Blue solid (2.14 g, quant.; mp 154–156 °C). IR (KBr) ν: 3482, 3093, 3058, 3025, 2948, 2827, 1598, 1450, 1342, 1157, 754 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, J = 8.4 Hz, 2H), 7.57 (d, J = 7.8 Hz, 1H), 7.31 (dd, J = 8.4, 8.4 Hz, 1H), 7.27–7.24 (m, 4H), 7.05 (d, J = 8.4 Hz, 1H), 6.85 (d, J = 8.4 Hz, 2H), 6.80 (dd, J = 7.2, 7.2 Hz, 1H), 5.59 (d, J = 1.2 Hz, 1H), 5.14 (d, J = 1.2 Hz, 1H), 3.62 (br s, 1H), 2.39 (s, 3H), 1.94 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 148.9, 145.1, 142.4, 135.4, 133.0, 131.5, 130.2, 129.3, 127.1, 125.8, 124.8, 118.0, 113.5, 112.8, 91.0, 67.1, 32.1, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{21}N_2O_3SNa$ 451.0859, 453.0830; Found 451.0855, 453.0828.

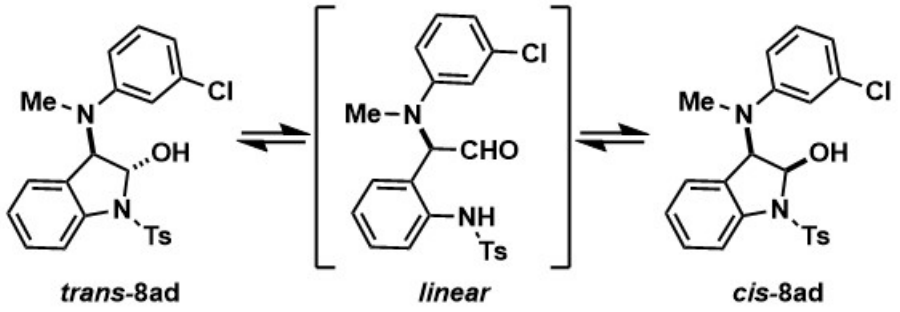


(*trans*:*cis* = 85:15)

(*rac*)-*trans*-7-Chloro-3-(methyl(phenyl)amino)-1-tosylindolin-2-ol (8ja).[4] To a solution of **S1j** (917 mg, 2 equiv., 3 mmol) and H_2O (0.54 mL, 20 equiv., 30 mmol) in acetone (15 mL, 0.2 M) was added NBS (587 mg, 2.2 equiv., 3.3 mmol). The mixture was stirred at room temperature for 9 h. Then Et_3N (0.46 mL, 2.2 equiv., 3.3 mmol) was added to the mixture and stirred further 1 h. The mixture was concentrated *in vacuo*. The residue was dissolved in AcOEt (15 mL, 0.1 M) and added *N*-methylaniline (161 mg, 1.5 mmol) and Et_3N (0.42 mL,

2.0 equiv., 3 mmol). The mixture was stirred at 80 °C in oil bath for 6 hours. 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 silica gel column chromatography using hexane/AcOEt (3/1 v/v) to give **8ja**.

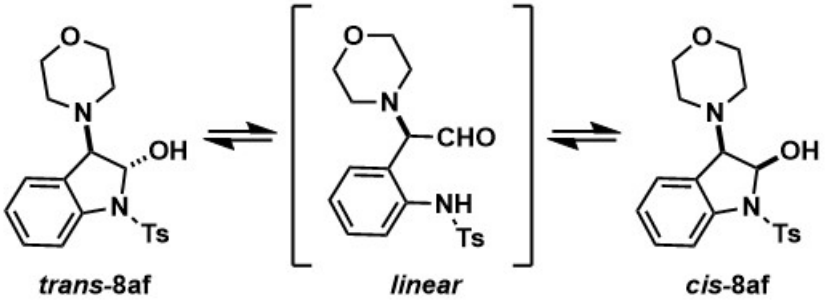
White solid (391 mg, 61% yield; mp 134–136 °C). IR (KBr) ν: 3423, 3064, 2979, 2923, 2813, 1600, 1506, 1461, 1328, 1147, 775 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, J = 8.4 Hz, 1.7H), 7.74 (d, J = 7.8 Hz, 0.30H), 7.34–7.25 (m, 5H), 7.19 (d, J = 7.2 Hz, 0.85H), 7.14 (dd, J = 7.8, 7.8 Hz, 0.15H), 7.08 (dd, J = 7.8, 7.8 Hz, 0.85H), 7.01 (d, J = 8.4 Hz, 1.85H), 6.87 (dd, J = 7.2, 7.2 Hz, 0.85H), 6.81 (dd, J = 7.2, 7.2 Hz, 0.15H), 6.64 (d, J = 8.4 Hz, 0.30H), 6.21 (s, 0.85H), 6.12 (d, J = 5.4 Hz, 0.15H), 5.09 (s, 0.85H), 5.03 (d, J = 6.0 Hz, 0.15H), 3.63 (br s, 0.85H), 3.22 (br s, 0.15H), 2.80 (s, 0.45H), 2.61 (s, 2.55H), 2.44 (s, 0.45H), 2.43 (2.55H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 149.5, 149.4, 144.7, 143.84, 143.84, 139.2, 138.9, 137.9, 136.9, 136.0, 133.0, 132.2, 131.2, 129.9, 129.61, 129.57, 129.50, 127.2, 127.0, 126.1, 126.0, 125.1, 123.9, 122.4, 118.7, 118.0, 114.3, 112.7, 90.6, 88.9, 67.3, 63.6, 36.0, 33.5, 21.8, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{21}N_2O_3SNa$ 451.0859, 453.0830; Found 451.0855, 453.0830.



trans*-8ad** ***linear ***cis*-8ad** (*tarns*:*cis* = 92:8)

(*rac*)-*trans*-3-((3-Chlorophenyl)(methyl)amino)-1-tosylindolin-2-ol (8ad).[3a] To a suspension of **S2a** (582 mg, 1.2 equiv., 1.2 mmol) in AcOEt (10 mL, 0.1 M) were added *m*-chloro-*N*-methylaniline (142 mg, 1.0 mmol) and Et_3N (0.26 mL, 2 equiv., 2.0 mmol). The suspension was stirred at 80 °C in oil bath for 2 h. After the whole was cooled to room temperature, H_2O (10 mL) was added to the mixture. The whole was 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 (2/1 v/v) to give **8ad**.

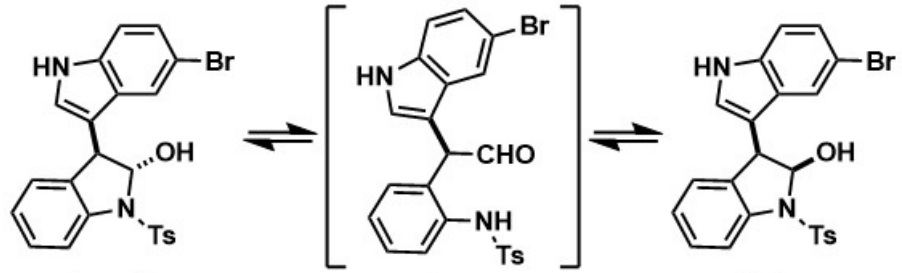
Purple oil (368 mg, 86% yield; mp 180 °C). IR (KBr) ν: 3471, 3064, 2948, 2900, 2817, 1592, 1496, 1346, 1160, 759 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 7.2 Hz, 1H), 7.36 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 7.25 (d, J = 8.4 Hz, 2H), 7.14 (dd, J = 8.4, 8.4 Hz. 1H), 7.11 (d, J = 7.2 Hz, 1H), 7.08 (dd, J = 7.8, 7.8 Hz, 1H), 6.84 (dd, J = 2.4, 2.4 Hz. 1H), 6.80 (dd, J = 8.4, 2.4 Hz, 1H), 6.77 (dd, J = 8.4, 1.2 Hz, 1H), 5.54 (d, J = 3.0 Hz, 1H), 5.15 (d, J = 2.4 Hz, 1H), 3.87 (br s, 1H), 2.38 (s, 3H), 1.91 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 150.5, 144.9, 140.9, 135.3, 135.2, 130.3, 130.3, 130.1, 127.4, 127.1, 126.3, 124.5, 118.2, 114.5, 113.9, 112.1, 90.2, 67.3, 33.0, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{21}ClN_2O_3SNa$ 451.0859, 453.0830; Found 451.0860, 453.0835.



trans-8af *linear* *cis*-8af (*trans*:*cis* = 92:8)

(*rac*)-*trans*-3-Morpholino-1-tosylindolin-2-ol (8af).[3a] To a suspension of **S2a** (582 mg, 1.2 equiv., 1.2 mmol) in AcOEt (10 mL, 0.1 M) were added morpholine (87 mg, 1.0 mmol) and Et_3N (0.26 mL, 2 equiv., 2.0 mmol). The suspension was stirred at 80 °C in oil bath for 2 h. After the whole was cooled to room temperature, H_2O (10 mL) was added to the mixture. The whole was 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 (2/1 v/v) to give **8af**.

White solid (276 mg, 74% yield; mp 164 °C). IR (KBr) ν: 3336, 2969, 2921, 2871, 2819, 1596, 1463, 1353, 1174, 1106, 765 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, J = 7.8 Hz, 2H), 7.57 (d, J = 8.4 Hz, 1H), 7.29 (dd, J = 7.8, 7.8 Hz, 1H), 7.26 (d, J = 7.8 Hz, 1H), 7.23 (d, J = 7.8 Hz, 2H), 7.05 (ddd, J = 7.2, 7.2, 0.6 Hz, 1H), 5.68 (d, J = 2.4 Hz, 1H), 4.07 (br s, 1H), 4.03 (d, J = 1.8 Hz, 1H), 3.49–3.46 (m, 2H), 3.44–3.40 (m, 2H), 2.34 (s, 3H), 2.15 (br s, 2H), 2.01 (br s, 2H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 1144.7, 140.9, 135.4, 129.95, 129.85, 127.6, 127.1, 126.8, 124.0, 114.1, 85.5, 72.9, 67.0, 48.8, 21.6. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{19}H_{22}N_2O_4SNa$ 397.1198; Found 397.1197.

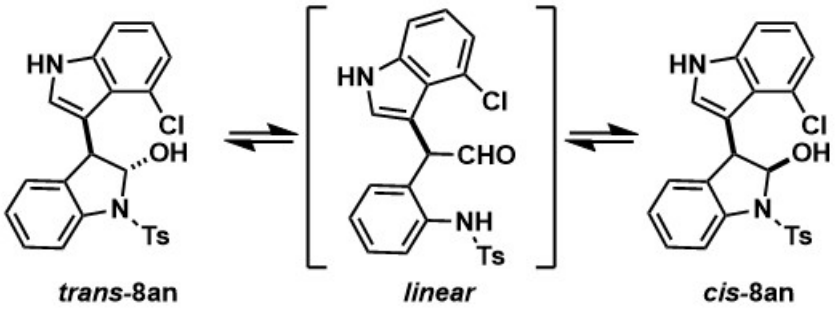


trans-8am *linear* *cis*-8am (*trans*:*cis* = 92:8)

(*rac*)-*trans*-3-(5-Bromo-1*H*-indol-3-yl)-1-tosylindolin-2-ol (8am).[3a] To a suspension of **S2a** (1.65 g, 1.2 equiv., 3.6 mmol) in AcOEt (30 mL, 0.1 M) were added 5-bromoindole (595 mg, 3.0 mmol) and Et_3N (0.83 mL, 2 equiv., 6.0 mmol). The suspension was stirred at 80 °C in oil bath for 2 h. After the whole was cooled to room temperature, H_2O (10 mL) was added to the mixture. The whole was 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 v/v) to give **8am**.

Brown oil (1.02 g, 70% yield). IR (KBr) ν: 3062, 2967, 2923, 1457, 1338, 1164, 750, 576 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.13 (br s, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.56 (d, J = 7.8 Hz, 2H), 7.28 (dd, J = 7.8, 7.8 Hz,

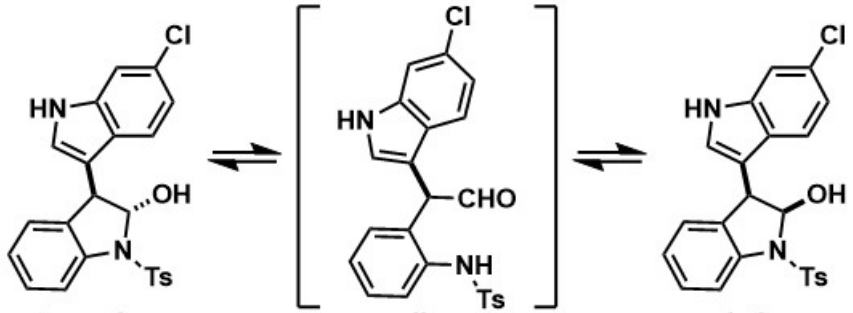
1H), 7.23 (dd, *J* = 9.0, 1.8 Hz, 1H), 7.18–7.17 (m, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 7.8 Hz, 1H), 7.01 (dd, *J* = 7.2, 7.2 Hz, 1H), 6.34 (s, 1H), 5.75 (dd, *J* = 3.0, 3.0 Hz, 1H), 4.52 (d, *J* = 1.8 Hz, 1H), 3.94 (d, *J* = 3.0 Hz, 1H), 2.33 (); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 144.5, 140.0, 135.3, 134.5, 131.0, 129.8, 128.7, 127.6, 127.1, 125.9, 125.s,3H4, 124.3, 124.0, 121.4, 114.6, 114.3, 113.1, 112.9, 93.0, 47.1, 21.8. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{19}BrN_2O_3SNa$ 505.0198, 507.0177; Found 505.0200, 507.0181.



trans-8an *linear* *cis*-8an (*trans*:*cis* = 81:19)

(*rac*)-*trans*-3-(4-Chloro-1*H*-indol-3-yl)-1-tosylindolin-2-ol (8am).[3a] To a suspension of **S2a** (1.65 g, 1.2 equiv., 3.6 mmol) in AcOEt (30 mL, 0.1 M) were added 4-chloroindole (455 mg, 3.0 mmol) and Et_3N (0.83 mL, 2 equiv., 6.0 mmol). The suspension was stirred at 80 °C in oil bath for 2 h. After the whole was cooled to room temperature, H_2O (10 mL) was added to the mixture. The whole was 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 v/v) to give **8an**.

Yellow oil (1.03 g, 78% yield). IR (KBr) ν: 3029, 2967, 2925, 1475, 1340, 1166, 750 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.46 (br s, 0.2H), 7.86 (br s, 0.8H), 7.82 (d, *J* = 8.4 Hz, 0.4H), 7.56 (d, *J* = 8.4 Hz, 1.6H), 7.54–7.53 (m, 1H), 7.28–7.23 (m, 1.6H), 7.18 (d, *J* = 7.8 Hz, 1.6H), 7.13–7.00 (m, 5H), 6.17 (dd, *J* = 6.6, 4.8 Hz, 0.2H), 5.91 (s, 0.8H), 5.61 (br s, 0.8H), 5.45 (d, *J* = 6.6 Hz, 0.2H), 5.05 (s, 0.8H), 3.39 (br s, 0.8H), 2.83 (d, *J* = 4.8 Hz, 0.2H), 2.38 (s, 0.6H), 2.33 (s, 2.4H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 144.4, 143.9, 140.4, 140.0, 138.0, 136.2, 135.5, 132.6, 132.2, 129.8, 129.4, 128.6, 128.4, 127.3, 126.8, 126.6, 126.0, 125.8, 125.7, 124.2, 124.1, 123.0, 122.9, 121.0, 120.8, 115.8, 114.8, 114.7, 110.8, 110.2, 108.7, 93.2, 87.7, 47.3, 44.8, 21.63, 21.57. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{19}N_2O_3SNa$ 461.0703, 463.0673; Found 461.0702, 463.0669.

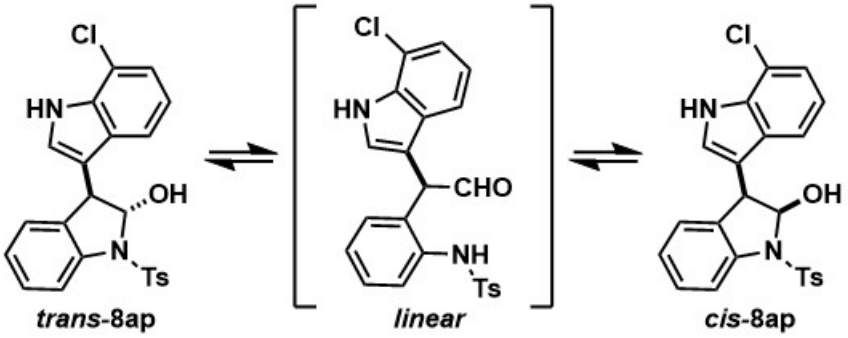


trans-8ao *linear* *cis*-8ao (*trans*:*cis* = 91:9)

(*rac*)-*trans*-3-(6-Chloro-1*H*-indol-3-yl)-1-tosylindolin-2-ol (8ao).[3a] To a suspension of **S2a** (1.65 g, 1.2 equiv., 3.6 mmol) in AcOEt (30 mL, 0.1 M) were added 6-chloroindole (455 mg, 3.0 mmol) and Et_3N (0.83 mL,

2 equiv., 6.0 mmol). The suspension was stirred at 80 °C in oil bath for 2 h. After the whole was cooled to room temperature, H_2O (10 mL) was added to the mixture. The whole was 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 v/v) to give **8ao**.

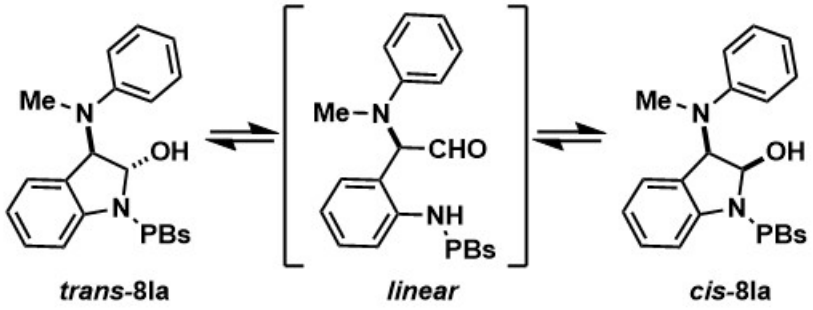
Yellow oil (1.14 g, 86% yield). IR (KBr) ν: 3384, 3064, 2965, 2877, 1596, 1459, 1340, 1166, 752, 578 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.01 (br s, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 8.4 Hz, 2H), 7.29–7.27 (m, 2H), 7.09 (d, J = 8.4 Hz, 2H), 7.03–6.98 (m, 2H), 6.74 (dd, J = 7.8, 1.8 Hz, 1H), 6.64 (d, J = 9.0 Hz, 1H), 6.48 (d, J = 2.4 Hz, 1H), 5.74 (d, J = 3.0 Hz, 1H), 4.53 (d, J = 3.0 Hz, 1H), 3.84 (br s, 1H), 2.37 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 144.6, 139.9, 137.1, 134.4, 131.3, 129.8, 128.7, 128.2, 127.2, 125.9, 124.34, 124.28, 123.6, 120.3, 119.6, 115.0, 114.2, 111.3, 92.9, 47.3, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{19}ClN_2O_3SNa$ 461.0703, 463.0673; Found 461.0700, 463.0674.



(*trans*:*cis* = 94:6)

(*rac*)-*trans*-3-(7-Chloro-1*H*-indol-3-yl)-1-tosylindolin-2-ol (8ap).[4] To a suspension of **S2a** (1.65 g, 1.2 equiv., 3.6 mmol) in AcOEt (30 mL, 0.1 M) were added 7-chloroindole (455 mg, 3.0 mmol) and Et_3N (0.83 mL, 2 equiv., 6.0 mmol). The suspension was stirred at 80 °C in oil bath for 2 h. After the whole was cooled to room temperature, H_2O (10 mL) was added to the mixture. The whole was 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 v/v) to give **8ap**.

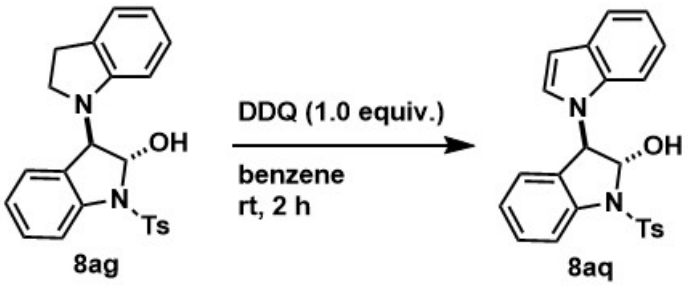
Pale-yellow oil (529 mg, 40% yield). IR (KBr) ν: 3064, 2956, 2923, 1596, 1477, 1346, 1166, 754, 576 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.09 (br s, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 7.8 Hz, 2H), 7.30 (ddd, J = 7.8, 7.8, 0.6 Hz, 1H), 7.15 (dd, J = 7.2, 1.8 Hz, 1H), 7.05–7.01 (m, 4H), 6.78–6.76 (m, 2H), 6.43 (d, J = 2.4 Hz, 1H), 5.76 (dd, J = 3.0, 3.0 Hz, 1H), 4.54 (d, J = 3.0 Hz, 1H), 3.87 (d, J = 3.0 Hz, 1H), 2.37 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 144.4, 140.0, 134.6, 134.0, 131.3, 129.7, 128.7, 127.2, 127.1, 125.9, 124.4, 123.4, 121.8, 120.5, 117.6, 116.7, 116.3, 114.6, 92.8, 47.3, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{19}ClN_2O_3SNa$ 461.0703, 463.0673; Found 461.0698, 463.0678.



trans-8la *linear* *cis*-8la (*trans*:*cis* = 99:1)

(*rac*)-*trans*-1-([1,1'-Biphenyl]-4-ylsulfonyl)-3-(methyl(phenyl)amino)indolin-2-ol (8la).[4] To a solution of **S1l** (1.00 g, 2 equiv., 3 mmol) and H_2O (0.54 mL, 20 equiv., 30 mmol) in acetone (15 mL, 0.2 M) was added NBS (587 mg, 2.2 equiv., 3.3 mmol). The mixture was stirred at room temperature for 21.5 h. Then Et_3N (0.46 mL, 2.2 equiv., 3.3 mmol) was added to the mixture and stirred further 1 h. The mixture was concentrated *in vacuo*. The residue was dissolved in AcOEt (15 mL, 0.1 M) and added *N*-methylaniline (161 mg, 1.5 mmol) and Et_3N (0.42 mL, 2.0 equiv., 3 mmol). The mixture was stirred at 80 °C in oil bath for 2 hours. 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 silica gel column chromatography using hexane/AcOEt (3/1 v/v) to give **8la**.

White solid (623 mg, 91% yield; mp 167–169 °C). IR (KBr) ν: 3467, 3064, 3029, 2950, 2817, 1600, 1504, 1355, 1164, 765, 609 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, J = 8.4 Hz, 2H), 7.71 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 9.0 Hz, 2H), 7.54 (d, J = 6.6 Hz, 2H), 7.47 (dd, J = 7.2, 7.2 Hz, 2H), 7.42 (dd, J = 7.2, 7.2 Hz, 1H), 7.38 (dd, J = 7.8, 7.8 Hz, 1H), 7.25 (dd, J =7.2, 7.2 Hz, 2H), 7.15 (d, J = 7.8 Hz, 1H), 7.10 (ddd, J = 7.2, 7.2, 0.6 Hz, 1H), 6.89 (d, J = 8.4 Hz, 2H), 6.81 (dd, J = 7.2, 7.2 Hz, 1H), 5.62 (dd, J = 2.4, 2.4 Hz, 1H), 5.22 (d, J = 1.8 Hz, 1H), 3.74 (d, J = 2.4 Hz, 1H), 1.96 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 149.3, 146.7, 140.8, 138.9, 136.8, 130.1, 129.5, 129.3, 128.9, 128.01, 128.01, 127.6, 127.4, 126.5, 124.5, 118.4, 114.5, 114.2, 90.2, 67.5, 33.1. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{27}H_{24}N_2O_3SNa$ 479.1405; Found 479.1403.



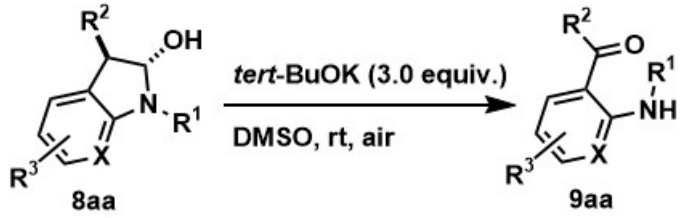
8ag 8aq (*trans*:*cis* = 96:4)

(*rac*)-*trans*-3-(1*H*-indol-1-yl)-1-tosylindolin-2-ol (8aq).[5] To a solution of **8ag** (582 mg, 1 mmol) in benzene (5 mL, 0.2 M) was added DDQ (227 mg, 1.0 equiv., 1 mmol). The mixture was stirred at room temperature for 2 h. After the whole was quenched with sat. $NaHCO_3$ (5 mL), the mixture 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

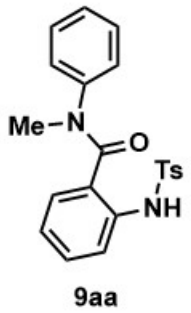
in vacuo. The residue was purified by silica gel column chromatography using hexane/AcOEt (3/1 v/v) to give **8aq**.

Pale-brown oil (406 mg, quant). IR (KBr) ν: 3048, 2923, 1596, 1457, 1353, 1166, 742, 576 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, J = 8.4 Hz, 1H), 7.622–7.608 (m, 1H), 7.615 (d, J = 8.4 Hz, 2H), 7.44 (dd, J = 7.8, 7.8 Hz, 1H), 7.16–7.07 (m, 7H), 6.25 (d, J = 3.0 Hz, 1H), 6.08 (br s, 1H), 5.77 (d, J = 1.8 Hz, 1H), 5.65 (s, 1H), 4.03 (d, J = 2.4 Hz, 1H), 2.42 (s, 3H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 144.8, 141.3, 135.9, 134.8, 130.8, 130.1, 129.5, 127.1, 126.7, 126.6, 125.1, 124.7, 122.0, 121.2, 120.3, 115.0, 109.9, 102.4, 91.9, 64.1, 21.5. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{20}N_2O_3SNa$ 427.1092; Found 427.1088.

Scheme S1. C1 deletion reactions of indoline hemiaminals

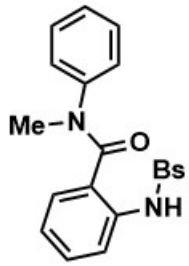


General Procedure: To a solution of **8** (0.5 mmol) in DMSO (2.5 mL, 0.2 M) was added *tert*-BuOK (168.3 mg, 1.5 mmol, 3.0 equiv.) under air condition. The mixture was stirred at room temperature until the complete disappearance of starting materials as indicated by TLC. After H_2O (20 mL) was added to the mixture, the whole was extracted with AcOEt (3 x 20 mL) and washed with brine (5 x 20 mL). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt solvent mixture as the eluent.



***N*-Methyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9aa).** The reaction was performed according to the general procedure used 394.5 mg (1 mmol) of **8aa**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9aa**.

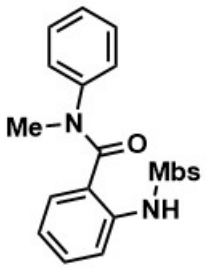
Pale-yellow solid (308 mg, 81% yield; mp 179–180 °C). IR (KBr) ν: 3226, 3062, 2983, 2958, 2917, 1623, 1583, 1484, 1369, 1166, 1089, 765, 563 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.33 (br s, 1H), 7.80 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz, 1H), 7.27 (d, J = 7.8 Hz, 2H), 7.16 (dd, J = 7.8, 7.8, 1.2 Hz, 1H), 7.09–7.04 (m, 3H), 6.66 (d, J = 7.8 Hz, 1H), 6.62 (dd, J = 7.2, 7.2 Hz, 1H), 6.35 (d, J = 6.0 Hz, 2H), 3.40 (s, 3H), 2.35 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 169.3, 144.3, 144.0, 137.4, 137.3, 131.0, 130.1, 129.8, 129.2, 127.6, 126.8, 126.3, 124.6, 123.0, 122.4, 38.5, 21.6. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{20}N_2O_3SNa$ 403.1092; Found 403.1091.



9ba

***N*-Methyl-*N*-phenyl-2-(phenylsulfonamido)benzamide (9ba).** The reaction was performed according to the general procedure used 190 mg (0.5 mmol) of **8ba**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ba**.

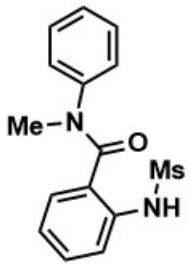
White solid (160 mg, 87% yield; mp 140–142 °C). IR (KBr) ν: 3235, 3058, 2942, 1629, 1590, 1488, 1376, 1168, 752, 582 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.42 (br s, 1H), 7.91 (d, J = 7.2 Hz, 2H), 7.65 (dd, J = 8.4, 1.2 Hz, 1H), 7.55–7.52 (m, 1H), 7.48 (dd, J = 7.8, 7.8 Hz, 2H), 7.15 (dd, J = 7.8, 7.8 Hz, 1H), 7.07–7.04 (m, 3H), 6.66 (d, J = 7.2 Hz, 1H), 6.62 (dd, J = 7.2, 7.2 Hz, 1H), 6.34 (br s, 2H), 3.38 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 169.2, 144.1, 140.3, 137.0, 133.2, 131.0, 130.1, 129.3, 129.2, 127.4, 126.8, 126.2, 124.6, 123.2, 122.5, 38.5. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{20}H_{18}N_2O_3SNa$ 389.0936; Found 389.0932.



9ca

2-((4-Methoxyphenyl)sulfonamido)-*N*-methyl-*N*-phenylbenzamide (9ca). The reaction was performed according to the general procedure used 205 mg (0.5 mmol) of **8ca**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ca**.

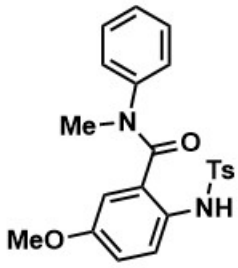
White solid (185 mg, 93% yield; mp 120–122 °C). IR (KBr) ν: 3280, 3056, 3008, 2975, 2940, 2902, 2840,1625, 1592, 1492, 1367, 1263, 1155, 755, 566 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.25 (br s, 1H), 7.84 (d, J = 7.8 Hz, 2H), 7.63 (d, J = 8.4 Hz, 1H), 7.14 (dd, J = 7.8, 7.8 Hz, 1H), 7.084–7.078 (m, 3H), 6.93 (d, J = 8.4 Hz, 2H), 6.68 (d, J = 7.8 Hz, 1H), 6.62 (dd, J = 7.2, 7.2 Hz, 1H), 6.46 (br s, 2H), 3.79 (s, 3H), 3.40 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 169.3, 163.3, 144.3, 137.4, 131.9, 131.0, 130.1, 129.6, 129.3, 126.8, 126.3, 124.5, 123.0, 122.2, 114.3, 55.7, 38.5. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{20}N_2O_4SNa$ 419.1042; Found 419.1038.



9da

***N*-Methyl-2-(methylsulfonamido)-*N*-phenylbenzamide (9da).** The reaction was performed according to the general procedure used 159 mg (0.5 mmol) of **8da**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9aa**.

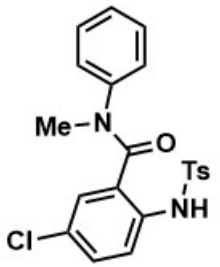
Pale-yellow oil (65.7 mg, 43% yield). IR (KBr) ν: 3262, 3064, 3029, 2931, 1627, 1592, 1494, 1330, 1155, 759, 700, 518 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.69 (br s, 1H), 7.55 (d, J = 8.4 Hz, 1H), 7.24 (dd, J = 7.8, 7.8 Hz, 2H), 7.21 (dd, J = 8.4, 8.4 Hz, 1H), 7.16 (dd, J = 7.2, 7.2 Hz, 1H), 7.03 (d, J = 7.8 Hz, 2H), 6.87 (d, J = 7.8 Hz, 1H), 6.72 (dd, J = 7.8, 7.8 Hz. 1H), 3.49 (s, 3H), 3.13 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 169.5, 144.3, 137.4, 131.1, 130.2, 129.6, 127.2, 126.5, 124.0, 122.7, 119.5, 40.4, 38.5. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{15}H_{16}N_2O_3SNa$ 327.0779; Found 327.0779.



9ea

5-Methoxy-*N*-methyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9ea). The reaction was performed according to the general procedure used 212 mg (0.5 mmol) of **8ea**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ea**.

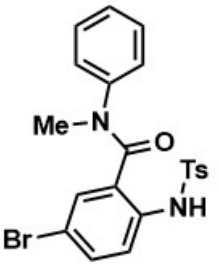
Pale-brown solid (134 mg, 60% yield; mp 116–118 °C). IR (KBr) ν: 3195, 3095, 3052, 3000, 2956, 2929, 2830,1621, 1589, 1496, 1367, 1268, 1160, 765, 701, 541 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.09 (br s, 1H), 7.76 (d, J = 7.8 Hz. 2H), 7.57 (d, J = 9.0 Hz, 1H), 7.27 (d, J = 9.0 Hz, 2H), 7.12–7.06 (m, 3H), 6.74 (dd, J = 9.0, 3.0 Hz, 1H), 6.26 (br s, 2H), 6.13 (br s, 1H), 3.38 (s, 3H), 3.28 (s, 3H), 2.34 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 168.7, 155.3, 144.4, 144.0, 137.5, 130.2, 129.7, 129.3, 127.7, 126.9, 126.3, 125.6, 117.9, 114.4, 55.3, 38.5, 21.6. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22,}H_{22}N_2O_4SNa$ 433.1195; Found 433.1198.



9fa

5-Chloro-*N*-methyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9fa). The reaction was performed according to the general procedure used 214 mg (0.5 mmol) of **8fa**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9fa**.

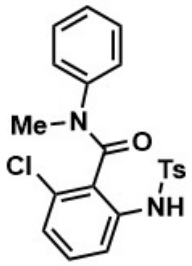
Pale-brown solid (156 mg, 75% yield; mp 163 °C). IR (KBr) ν: 3266, 3056, 2927, 2877, 1631, 1589, 1492, 1375, 1166, 1091, 767, 700, 570 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.19 (br s, 1H), 7.79 (d, J = 8.4 Hz, 2H), 7.60 (d, J = 8.4 Hz, 1H), 7.29 (d, J = 7.8 Hz, 2H), 7.16–7.10 (m, 4H), 6.61 (br s, 1H), 6.37 (br s, 2H), 3.40 (s, 3H), 2.37 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 167.9, 144.3, 143.8, 137.2, 135.9, 131.0, 129.94, 129.94, 129.5, 128.7, 127.6, 127.4, 126.3, 125.9, 123.8, 38.5, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{19}ClN_2O_3SNa$ 437.0703, 439.0673; Found 437.0701, 439.0678.



9ga

5-Bromo-*N*-methyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9ga). The reaction was performed according to the general procedure used 236 mg (0.5 mmol) of **8ga**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ga**.

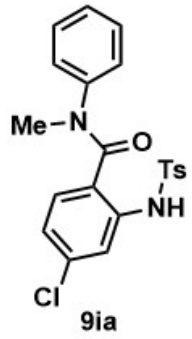
White solid (134 mg, 58% yield; mp 161–163 °C). IR (KBr) ν: 3270, 3052, 3031, 2925, 2877, 1646, 1590, 1492, 1328, 1166, 1089, 763, 703, 578 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.20 (br s, 1H), 7.78 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 9.0 Hz, 1H), 7.29 (d, J = 8.4 Hz, 2H), 7.26–7.25 (m, 1H), 7.15 (dd, J = 7.8, 7.8 Hz, 1H), 7.11 (dd, J = 7.2, 7.2 Hz, 2H), 6.76 (br s, 1H), 6.38 (br s, 2H), 3.39 (s, 3H), 2.37 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 167.7, 144.3, 143.8, 137.1, 136.3, 133.8, 132.9, 129.9, 129.5, 127.6, 127.4, 126.3, 126.1, 123.9, 116.0, 38.5, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{19}BrN_2O_3SNa$ 481.0198, 483.0177; Found 481.0201, 483.0177.



9ha (containing rotamer)

4-Chloro-*N*-methyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9ha). The reaction was performed according to the general procedure used 214 mg (0.5 mmol) of **8ha**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ha**.

White solid (167 mg, 81% yield; mp 150–153 °C, containing rotamer). IR (KBr) ν: 3280, 3116, 3052, 2954, 2923, 2877, 1639, 1592, 1492, 1369, 1168, 1091, 941, 769, 700, 543 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, J = 9.0 Hz, 1.5H), 7.77 (d, J = 9.0 Hz, 0.50H), 7.68 (br s, 0.75H), 7.56 (d, J = 8.4 Hz, 0.25H), 7.47 (dd, J = 7.2, 7.2 Hz, 0.5H), 7.42 (br s, 0.25H), 7.35 (ddd, J = 7.2, 7.2, 1.2 Hz, 0.25H), 7.31–7.28 (m, 3.5H), 7.20 (dd, J = 8.4, 1.2 Hz, 0.25H), 7.12–7.07 (m, 2.25H), 6.99 (dd, 8.4, 8.4 Hz, 0.75H), 6.90 (d, J = 7.8 Hz. 1.5H), 6.72 (d, J = 6.6 Hz, 0.75H), 3.51 (s, 2.25H), 2.84 (s, 0.75H), 2.39 (s, 0.75H), 2.38 (s, 2.25H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 166.4, 166.1, 144.6, 144.5, 142.1, 142.0, 137.2, 137.0, 136.4, 135.6, 131.1, 130.9, 130.7, 130.6, 130.1, 130.0, 129.6, 128.7, 128.5, 127.8, 127.5, 127.46, 127.46, 126.6, 126.2, 126.1, 125.9, 124.6, 121.6, 116.9, 39.0, 37.4, 21.71, 21.68. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{19}ClN_2O_3SNa$ 437.0703, 439.0673; Found 437.0702, 439.0677.

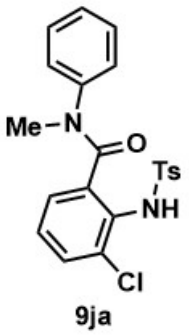


9ia

6-Chloro-*N*-methyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9ia). The reaction was performed according to the general procedure used 214 mg (0.5 mmol) of **8ia**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ia**.

Pale-yellow solid (163 mg, 79% yield; mp 164 °C). IR (KBr) ν: 3147, 3089, 2985, 2946, 2921, 1621, 1583, 1492, 1326, 1164, 935, 767, 713, 563 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.43 (br s, 1H), 7.82 (d, J = 7.8 Hz, 2H), 7.69 (d, J =1.8 Hz, 1H), 7.31 (d, J = 8.4 Hz ,2H), 7.12 (dd, J = 7.2, 7.2 Hz, 1H), 7.09 (dd, J = 7.8, 7.8 Hz, 2H), 6.59 (d, J = 8.4 Hz, 1H), 6.56 (d, J = 8.4 Hz, 1H), 6.37 (d, J = 7.2 Hz .1H), 3.4 (s, 3H), 2.38 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 168.6, 144.4, 144.1, 138.8, 137.1, 137.0, 131.1, 130.0, 129.5, 127.6, 127.1, 126.3, 123.2, 122.5, 122.2, 38.6, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{19}ClN_2O_3SNa$ 437.0703,

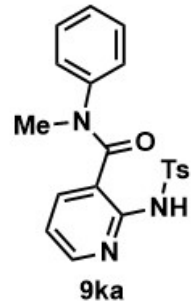
439.0673; Found 437.0708, 439.0677.



9ja

7-Chloro-*N*-methyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9ja). The reaction was performed according to the general procedure used 214 mg (0.5 mmol) of **8ja**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ja**.

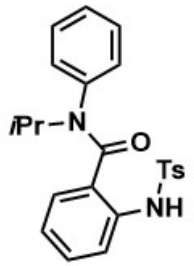
Pale-yellow oil (134 mg, 63% yield). IR (KBr) ν: 3062, 3031, 2917, 2859, 2840, 1627, 1592, 1496, 1336, 1155, 1091, 935, 806, 703, 665, 499 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, J = 8.4 Hz, 2H), 7.45 (br s, 1H), 7.36–7.09 (m, 9H), 6.95 (dd, J = 7.2, 7.2 Hz, 1H), 2.99 (s, 3H), 2.40 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 167.9, 144.03, 144.03, 143.8, 137.1, 135.3, 132.8, 131.43, 131.36, 129.5, 129.0, 128.9, 127.58, 127.58, 127.2, 126.7, 38.0, 21.6. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{19}ClN_2O_3SNa$ 437.0703, 439.0673; Found 437.0704, 439.0678.



9ka

***N*-Methyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylnicotinamide (9ka).** The reaction was performed according to the general procedure used 197 mg (0.5 mmol) of **8ka**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ka**.

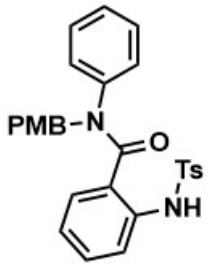
Pale-brown oil (70.7 mg, 37% yield). IR (KBr) ν: 3218, 3087, 3037, 2925, 1650, 1581, 1494, 1280, 1141, 1085, 773, 566 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.58 (br s, 1H), 8.06 (br s 1H), 8.04 (d, J = 6.6 Hz, 2H), 7.27 (d, J = 7.8 Hz, 2H), 7.26–7.23 (m, 2H), 7.19 (dd, J = 7.2, 7.2 Hz, 1H), 7.004–6.992 (m, 1H), 6.998 (d, J = 7.2 Hz, 2H), 6.48 (br s, 1H), 3.48 (s, 3H), 2.39 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 168.2, 150.6, 149.4, 144.0, 143.8, 138.3, 137.5, 129.8, 129.3, 128.5, 127.5, 126.7, 116.7, 116.1, 38.7, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{20}H_{19}N_3O_3SNa$ 404.1045; Found 404.1043.



9ab

***N*-Isopropyl-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9ab).** The reaction was performed according to the general procedure used 211 mg (0.5 mmol) of **8ab**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ab**.

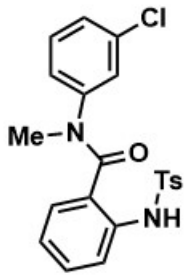
Pale-yellow solid (187 mg, 92% yield; mp 120–123 °C). IR (KBr) ν: 3218, 3062, 3029, 2969, 2933, 2877, 1617, 1589, 1488, 1376, 1159, 1093, 761, 705, 565 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.18 (br s, 1H), 7.77 (d, J = 8.4 Hz, 2H), 7.60 (dd, J = 8.4, 0.6 Hz, 1H), 7.27 (d, J = 8.4 Hz, 2H), 7.10 (dd, J = 7.8, 7.8 Hz, 1H), 7.06 (dd, J = 7.2, 7.2 Hz, 1H), 7.02 (dd, J = 7.8, 7.8 Hz, 2H), 6.67 (d, J = 6.0 Hz, 1H), 6.57 (dd, J = 7.2, 7.2 Hz, 1H), 6.31 (br s, 2H), 4.94 (br s, 1H), 2.37 (s, 3H), 1.13 (d, J = 7.2 Hz, 6H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 169.2, 143.9, 139.3, 137.7, 136.7, 130.4, 129.9, 129.7, 128.7, 127.6, 127.4, 125.7, 122.8, 121.7, 48.6, 21.6, 20.9. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{24}N_2O_3SNa$ 431.1405; Found 431.1403.



9ac

***N*-(4-Methoxybenzyl)-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9ac).** The reaction was performed according to the general procedure used 250 mg (0.5 mmol) of **8ac**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ac**.

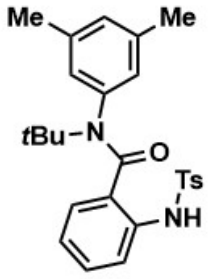
Pale-yellow solid (201 mg, 83% yield; mp 128–130 °C). IR (KBr) ν: 3237, 3073, 3045, 2996, 2948, 2836, 1621, 1585, 1488, 1380, 1245, 1162, 1031, 910, 754, 703, 565 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.47 (br s, 1H), 7.72 (dd, J = 8.4, 0.6 Hz, 1H), 7.59 (d, J = 8.4 Hz. 2H), 7.14–7.11 (m, 3H), 7.04 (dd, J = 7.8, 7.8 Hz, 1H), 6.97 (d, J = 8.4 Hz, 2H), 6.94 (dd, J = 7.8, 7.8 Hz, 2H), 6.85 (d, J = 8.4 Hz , 2H), 6.69 (d, J = 7.2 Hz, 1H), 6.59 (dd, J = 7.2, 7.2 Hz, 1H), 6.04 (d, J = 7.2 Hz, 2H), 4.95 (s, 2H), 3.80 (s, 3H), 2.25 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 168.9, 159.2, 143.7, 142.5, 137.3, 137.1, 130.9, 130.5, 130.1, 129.7, 129.0, 128.6, 127.3, 127.2, 126.8, 124.7, 123.1, 122.6, 113.7, 55.3, 53.3, 21.4. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{28}H_{26}N_2O_4SNa$ 509.1511; Found 509.1511.



9ad

***N*-Chloro-2-((4-methylphenyl)sulfonamido)-*N*-phenylbenzamide (9ad).** The reaction was performed according to the general procedure used 214 mg (0.5 mmol) of **8ad**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ad**.

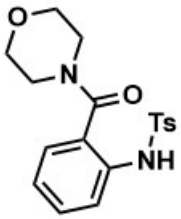
Brown oil (126 mg, 50% yield). IR (KBr) ν: 3208, 3079, 2956, 2913, 1627, 1585, 1486, 1361, 1166, 1089, 763, 715 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.27 (br s, 1H), 7.79 (d, J = 7.8 Hz, 2H), 7.65 (d, J = 7.8 Hz, 1H), 7.27 (d, J = 7.8 Hz, 2H), 7.21 (dd, J = 7.8, 7.8 Hz, 1H), 7.08 (d, J = 7.8 Hz, 1H), 6.97 (dd, J = 8.4, 8.4 Hz, 1H), 6.71–6.66 (m, 2H), 6.51 (s, 1H), 6.18 (d, J = 6.6 Hz, 1H), 3.39 (s, 3H), 2.34 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 169.1, 145.4, 144.1, 137.32, 137.32, 134.7, 131.4, 129.96, 129.96, 130.0, 127.5, 127.1, 126.21, 126.21, 124.7, 123.3, 123.0, 38.6, 21.6. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{19}ClN_2O_3SNa$ 437.0703, 439.0673; Found 437.0698, 439.0671.



9ae

***N*-(*tert*-Butyl)-*N*-(3,5-dimethylphenyl)-2-((4-methylphenyl)sulfonamido)benzamide (9ae).** The reaction was performed according to the general procedure used 232 mg (0.5 mmol) of **8ae**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ae**.

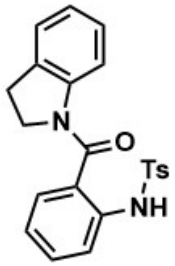
White solid (317 mg, 70% yield; mp 149 °C). IR (KBr) ν: 3166, 2979, 2960, 2921, 2863, 1617, 1587, 1486, 1367, 1267, 1160, 1093, 937, 759, 715 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.66 (br s, 1H), 7.85 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 8.4 Hz, 2H), 7.28 (dd, J = 7.8, 0.6 Hz, 1H), 6.94 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 6.79 (dd, J = 7.8, 1.2 Hz, 1H), 6.72 (s, 1H), 6.58 (ddd, J = 7.2, 7.2, 0.6 Hz, 1H), 6.42 (s, 2H), 2.40 (s, 3H), 2.12 (s, 6H), 1.49 (s, 9H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 170.4, 143.7, 140.9, 138.1, 137.8, 135.6, 129.9, 129.5, 129.4, 128.8, 128.1, 127.8, 127.4, 122.2, 119.5, 59.5, 29.2, 21.7, 21.1. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{26}H_{30}N_2O_3SNa$ 473.1875; Found 473.1877.



9af

4-Methyl-*N*-(2-(morpholine-4-carbonyl)phenyl)benzenesulfonamide (9af). The reaction was performed according to the general procedure used 187 mg (0.5 mmol) of **8af**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9af**.

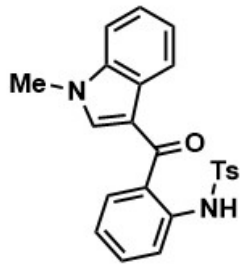
Pale-yellow oil (136 mg, 76% yield). IR (KBr) ν: 3216, 3064, 2965, 2921, 2857, 1619, 1596, 1490, 1338, 1164, 763, 721, 565 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.51 (br s, 1H), 7.65 (d, J = 7.8 Hz, 2H), 7.62 (dd, J = 8.4, 1.2 Hz, 1H), 7.36 (dd, J = 7.2, 7.2 Hz, 1H), 7.21 (d, J = 7.8 Hz, 2H), 7.09–7.06 (m, 2H), 3.61–3.11 (m, 8H), 2.36 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 168.4, 143.9, 137.0, 136.4, 131.3, 129.7, 127.8, 127.2, 125.0, 124.1, 123.7, 66.6, 48.3, 42.5, 21.5. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{18}H_{20}N_2O_4SNa$ 383.1042; Found 383.1042.



9ag

***N*-(2-(Indoline-1-carbonyl)phenyl)-4-methylbenzenesulfonamide (9ag).** The reaction was performed according to the general procedure used 203 mg (0.5 mmol) of **8ag**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ag**.

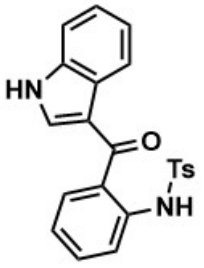
Colorless oil (128 mg, 65% yield). IR (KBr) ν: 3251, 3064, 3031, 2958, 2923, 2857, 1625, 1589, 1482, 1338, 1164, 759, 563 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.67 (s, 1H), 8.16 (br s, 1H), 7.73 (d, J = 7.2 Hz, 1H), 7.54 (d, J = 7.8 Hz, 2H), 7.42 (dd, J = 7.8, 7.8 Hz, 1H), 7.26–7.08 (m, 5H), 6.90 (d, J = 7.8 Hz, 2H), 3.43 (br s, 2H), 2.87 (br s, 2H), 2.19 (br s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 167.0, 143.6, 141.9, 136.6, 135.7, 131.9, 131.6, 129.44, 129.44, 127.1, 126.9, 125.6, 124.83, 124.83, 118.2, 115.5, 50.8, 28.1, 21.5. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{20}N_2O_3SNa$ 415.1092; Found 415.1095.



9ah

4-Methyl-*N*-(2-(1-methyl-1*H*-indole-3-carbonyl)phenyl)benzenesulfonamide (9ah). The reaction was performed according to the general procedure used 209 mg (0.5 mmol) of **8ah**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ah**.

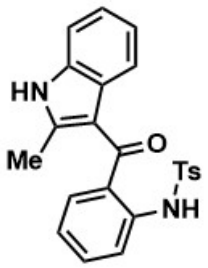
Pale-yellow oil (272 mg, 67% yield). IR (KBr) ν: 3205, 3054, 3029, 2921, 1606, 1521, 1365, 1164, 754, 561 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.62 (br s, 1H), 8.20 (d, J = 7.8 Hz, 1H), 7.72 (dd, J = 8.4, 1.2 Hz, 1H), 7.53 (dd, J = 7.8, 1.8 Hz, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.45 (ddd, J = 7.8, 7.8, 1.8 Hz, 1H), 7.37–7.32 (m, 3H), 7.16 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 7.09 (s, 1H), 6.79 (d, J = 7.8 Hz, 2H), 3.80 (s, 3H), 2.04 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 190.8, 143.1, 138.5, 137.4, 137.1, 136.2, 132.1, 130.6, 130.3, 129.2, 127.3, 127.0, 124.1, 124.03, 123.95, 123.1, 122.7, 115.8, 109.8, 33.7, 21.3. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{20}N_2O_3SNa$ 427.1092; Found 417.1092.



9ai

***N*-(2-(1*H*-Indole-3-carbonyl)phenyl)-4-methylbenzenesulfonamide (9ai).** The reaction was performed according to the general procedure used 202 mg (0.5 mmol) of **8ai**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ai**.

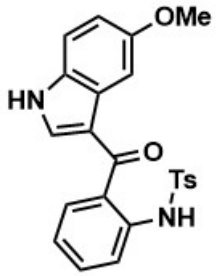
Pale-brown (138 mg, 71% yield). IR (KBr) ν: 3338, 3122, 3060, 2923, 2867, 1606, 1488, 1428, 1386, 1330, 1195, 1160, 923, 754, 719, 561 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.69 (s, 1H), 9.56 (br s, 1H), 8.22–8.20 (m, 1H), 7.71 (dd, J = 8.4, 1.2 Hz, 1H), 7.53 (dd, J = 7.8, 1.8 Hz, 1H), 7.47 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 7.444–7.430 (m, 1H), 7.437 (d, J = 8.4 Hz, 2H), 7.31–7.29 (m, 2H), 7.17 (d, J = 3.0 Hz, 1H), 7.16 (ddd, J = 7.8, 7.8, 0.6 Hz, 1H), 6.74 (d, J = 7.8 Hz, 2H), 2.03 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 191.6, 143.8, 136.7, 136.4, 135.41, 135.37, 132.2, 130.8, 130.6, 129.5, 127.2, 126.1, 124.7, 124.27, 124.27, 123.1, 122.2, 116.8, 112.0, 21.3. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{18}N_2O_3SNa$ 413.0936; Found 413.0936.



9aj

4-Methyl-*N*-(2-(2-methyl-1*H*-indole-3-carbonyl)phenyl)benzenesulfonamide (9aj). The reaction was performed according to the general procedure used 209 mg (0.5 mmol) of **8aj**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9aj**.

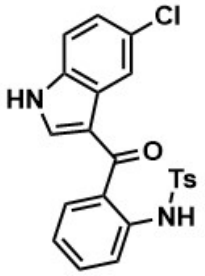
Pale-brown oil (55.1 mg, 50% yield). IR (KBr) ν: 3336, 3056, 2921, 1606, 1486, 1378, 1159, 763, 561 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 10.00 (s, 1H), 8.90 (br s,1H), 7.80 (dd, J =9.0, 1.2 Hz, 1H), 7.57 (d, J = 8.4 Hz, 2H), 7.47 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 7.46 (d, J = 7.8 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H), 7.14 (ddd, J = 7.8, 7.8, 0.6 Hz, 1H), 7.06 (ddd, J = 7.2, 7.2, 1.2 Hz, 1H), 6.95 (ddd, J = 7.8, 7.8, 0.6 Hz, 1H), 6.89 (d, J = 8.4 Hz, 2H), 6.76 (d, J = 7.8 Hz, 1H), 2.42 (s, 3H), 2.03 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 193.4, 144.7, 143.8, 137.3, 135.9, 134.6, 132.9, 132.4, 130.0, 129.6, 127.2, 127.1, 124.2, 123.4, 122.7, 121.6, 120.9, 114.0, 110.9, 21.3, 14.6. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{20}N_2O_3SNa$ 427.1092; Found 427.1089.



9ak

***N*-(2-(5-Methoxy-1*H*-indole-3-carbonyl)phenyl)-4-methylbenzenesulfonamide (9ak).** The reaction was performed according to the general procedure used 435 mg (0.5 mmol) of **8ak**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ak**.

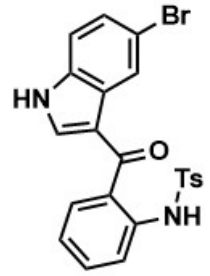
Brown oil (86.4 mg, 41% yield). IR (KBr) ν: 3359, 3064, 2996, 2935, 2832, 1594, 1486, 1380, 1272, 1159, 1089, 811, 717, 561 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.60 (s, 1H), 8.95 (br s, 1H), 7.72 (s, 1H), 7.70 (d, J = 7.8 Hz, 1H), 7.52 (d, J = 6.6 Hz, 1H), 7.48 (d, J = 7.2 Hz, 2H), 7.45 (dd, J = 7.2, 7.2 Hz, 1H), 7.31 (d, J = 7.8 Hz, 1H), 7.18–7.14 (m, 2H), 6.95 (d, J = 6.6 Hz, 1H), 6.80 (d, J = 7.2 Hz, 2H), 3.90 (s, 3H), 2.07 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 191.4, 156.7, 156.7, 143.5, 137.0, 135.9, 135.0, 132.1, 131.0, 130.6, 130.4, 129.4, 127.3, 127.1, 124.3, 124.0, 117.0, 114.8, 112.5, 103.7, 55.9, 21.4. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{20}N_2O_4SNa$ 443.1042; Found 443.1039.



9al

***N*-(2-(5-Chloro-1*H*-indole-3-carbonyl)phenyl)-4-methylbenzenesulfonamide (9al).** The reaction was performed according to the general procedure used 219 mg (0.5 mmol) of **8al**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9al**.

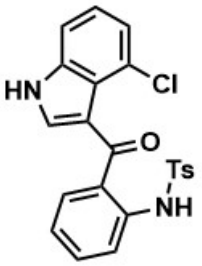
Brown oil (153 mg, 72% yield). IR (KBr) ν: 3289, 3031, 2923, 1608, 1517, 1326, 1160, 883, 761, 561 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.635 (s, 1H), 9.635 (br s, 1H), 8.14 (d, J = 1.2 Hz, 1H), 7.68 (d, J = 8.4 Hz, 1H), 7.52 (d, J = 7.2 Hz, 1H), 7.47 (dd, J = 7.8 Hz, 1H), 7.44 (d, J= 7.8 Hz, 2H), 7.36 (d, J = 8.4 Hz, 1H), 7.23 (d, J = 7.8 Hz, 1H), 7.21 (s, 1H), 7.17 (dd, J = 7.2, 7.2 Hz, 1H), 6.79 (d, J = 7.8 Hz, 2H), 2.04 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 191.3, 143.9, 136.8, 136.0, 135.4, 134.7, 132.4, 130.7, 130.2, 129.5, 128.9, 127.2, 124.7, 124.6, 124.3, 121.77, 121.77, 116.4, 113.0, 21.3. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{17}ClN_2O_3SNa$ 447.0546, 449.0517; Found 447.0551, 449.0514.



9am

***N*-(2-(5-Bromo-1*H*-indole-3-carbonyl)phenyl)-4-methylbenzenesulfonamide (9am).** The reaction was performed according to the general procedure used 242 mg (0.5 mmol) of **8am**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9am**.

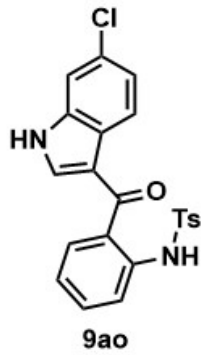
Brown oil (125 mg, 53% yield). IR (KBr) ν: 3255, 3029, 2923, 2850, 1608, 1517, 1428, 1328, 1159, 761, 719, 559 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.61 (s, 1H), 8.86 (br s, 1H), 8.28 (s, 1H), 7.73 (d, J = 7.8 Hz, 1H), 7.540–7.528 (m, 1H), 7.534 (d, J = 7.2 Hz, 2H), 7.48 (dd, J = 7.2, 7.2 Hz, 1H), 7.42 (d, J = 5.4 Hz, 1H), 7.32–7.26 (m, 2H), 7.16 (dd, J = 6.0, 6.0 Hz, 1H), 6.88 (d, J = 7.2 Hz, 2H), 2.10 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 191.3, 143.9, 136.9, 135.7, 135.5, 135.0, 132.5, 130.8, 130.1, 129.5, 127.7, 127.2, 124.86, 124.86, 124.6, 124.2, 116.6, 116.4, 113.4, 21.4. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{17}BrN_2O_3SNa$ 491.0041, 493.0021; Found 491.0041, 493.0020.



9an

***N*-(2-(4-Chloro-1*H*-indole-3-carbonyl)phenyl)-4-methylbenzenesulfonamide (9an).** The reaction was performed according to the general procedure used 219 mg (0.5 mmol) of **8an**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9an**.

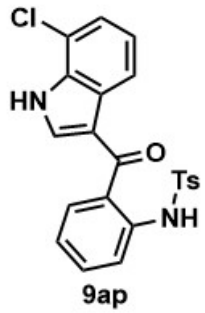
Brown oil (43.9 mg, 21% yield). IR (KBr) ν: 3212, 3118, 3064, 3029, 2923, 2854, 1608, 1488, 1338, 1159, 1089, 734, 565 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 10.89 (s, 1H), 8.91 (br s, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.72 (d, J = 7.8 Hz, 2H), 7.55 (d, J = 7.2 Hz, 1H), 7.45 (dd, J = 7.8, 7.8 Hz, 1H), 7.36 (br s, 1H), 7.22–7.20 (m, 3H), 7.15 (d, J = 7.8 Hz, 2H), 6.99 (dd, J = 7.8, 7.8 Hz, 1H), 2.33 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 193.3, 143.9, 139.5, 137.6, 136.7, 134.02, 133.99, 131.8, 129.8, 127.5, 126.9, 126.8, 124.7, 123.9, 123.5, 122.9, 120.5, 117.9, 110.6, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{17}ClN_2O_3SNa$ 447.0546, 449.0517; Found 447.0544, 449.0518.



9ao

***N*-(2-(6-Chloro-1*H*-indole-3-carbonyl)phenyl)-4-methylbenzenesulfonamide (9ao).** The reaction was performed according to the general procedure used 219 mg (0.5 mmol) of **8ao**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ao**.

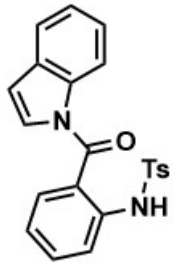
Pale-brown oil (72.9 mg, 34% yield). IR (KBr) ν: 3272, 3064, 2969, 2923, 2854, 1608, 1515, 1330, 1160, 1089, 879, 761, 727, 566 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.66 (s, 1H), 9.59 (br s, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.68 (dd, J = 8.4, 1.2 Hz, 1H), 7.52 (dd, J = 7.8, 1.2 Hz, 1H), 7.47 (dd, J = 7.2, 7.2 Hz, 1H), 7.45 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 1.2 Hz, 1H), 7.24 (dd, J = 7.8, 1.8 Hz. 1H), 7.18 (d, J = 2.4 Hz, 1H), 7.16 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 6.80 (d, J = 8.4 Hz, 2H), 2.06 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 191.4, 143.9, 136.82, 136.75, 135.6, 135.4, 132.5, 130.8, 130.1, 130.0, 129.5, 127.2, 124.66, 124.66, 124.1, 123.7, 123.2, 116.7, 111.9, 21.3. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{17}ClN_2O_3SNa$ 447.0546, 449.0517; Found 447.0544, 449.0522.



9ap

***N*-(2-(7-Chloro-1*H*-indole-3-carbonyl)phenyl)-4-methylbenzenesulfonamide (9ap).** The reaction was performed according to the general procedure used 219 mg (0.5 mmol) of **8ap**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9ap**.

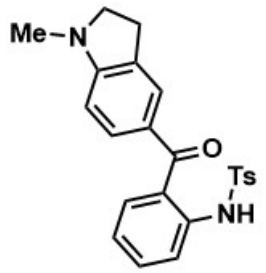
Pale-yellow oil (99.8 mg, 47% yield). IR (KBr) ν: 3261, 3060, 2921, 2856, 1614, 1587, 1430, 1386, 1166, 1083, 759, 547 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.50 (s, 1H), 9.06 (br s, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.74 (d, J = 8.4 Hz, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.49 (dd, J = 7.8, 7.8 Hz, 1H), 7.46 (d, J = 7.8 Hz, 2H), 7.34 (d, J = 7.2 Hz. 1H), 7.27–7.24 (m,.2H), 7.18 (dd, J = 7.2, 7.2 Hz, 1H), 6.78 (d, J = 7.8 Hz, 2H), 2.06 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 191.4, 143.4, 137.1, 135.9, 134.6, 133.5, 132.5, 130.5, 130.2, 129.4, 127.6, 127.4, 124.6, 124.5, 124.0, 123.7, 121.2, 118.1, 117.0, 21.3. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{17}ClN_2O_3SNa$ 447.0546, 449.0517; Found 447.0546, 449.0519.



9aq

***N*-(2-(1*H*-Indole-1-carbonyl)phenyl)-4-methylbenzenesulfonamide (9aq).** The reaction was performed according to the general procedure used 202 mg (0.5 mmol) of **8aq**. Purification by column chromatography on silica gel using hexane/AcOEt (3/1 v/v) to give **9aq**.

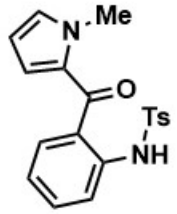
Pale-yellow solid (121 mg, 62% yield). IR (KBr) ν: 3278, 3151, 3110, 3064, 3050, 3029, 2973, 2917, 1652, 1600, 1452, 1338, 1162, 767, 559 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 8.54 (s, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.82 (dd, J = 8.4, 1.2 Hz, 1H), 7.58–7.56 (m, 2H), 7.45 (d, J = 8.4 Hz, 2H), 7.38 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 7.35–7.32 (m, 2H), 7.24 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 6.77 (d, J = 7.8 Hz, 2H), 6.63 (d, J = 3.6 Hz, 1H), 6.46 (d, J= 3.0 Hz, 1H), 2.05 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 167.4, 144.0, 137.4, 135.74, 135.66, 133.1, 130.7, 130.3, 129.5, 127.4, 127.0, 126.6, 126.0, 125.4, 125.0, 124.6, 121.0, 116.6, 108.9, 21.4. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{18}N_2O_3SNa$ 413.0936; Found 413.0937.



9ar

4-Methyl-*N*-(2-(1-methylindoline-5-carbonyl)phenyl)benzenesulfonamide (9ar). The reaction was performed according to the general procedure used 210 mg (0.5 mmol) of **8ar**. Purification by column chromatography on silica gel using hexane/AcOEt (1/1 v/v) to give **9ar**.

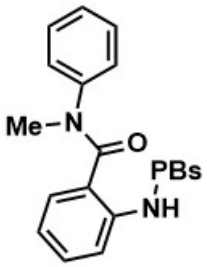
Pale-yellow oil (113 mg, 56% yield). IR (KBr) ν: 3174, 3056, 2952, 2921, 2836, 1589, 1338, 1162 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.49 (s, 1H), 7.73 (dd, J = 8.4, 1.2 Hz. 1H), 7.49 (d, J = 8.4 Hz, 2H), 7.44 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 7.33 (dd, J = 7.8, 1.2 Hz, 1H), 7.26 (s, 1H), 7.12–7.08 (m, 2H), 6.96 (d, J = 7.8 Hz, 2H), 6.20 (d, J = 9.0 Hz, 1H), 3.55 (t, J = 8.4 Hz, 2H), 3.00 (t, J = 8.4 Hz, 2H), 2.88 (s, 3H), 2.18 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 195.3, 157.2, 143.3, 137.8, 136.0, 133.8, 132.2, 131.8, 129.6, 129.5, 129.3, 127.3, 126.5, 125.9, 124.1, 123.7, 103.8, 55.0, 34.2, 27.7, 21.5. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{22}N_2O_3SNa$ 429.1249; Found 429.1246.



9as

4-Methyl-*N*-(2-(1-methyl-1*H*-pyrrole-2-carbonyl)phenyl)benzenesulfonamide (9as). The reaction was performed according to the general procedure used 184 mg (0.5 mmol) of **8as**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9as**.

Pale-yellow oil (120 mg, 68% yield). IR (KBr) ν: 3216, 3064, 2950, 2925, 1608, 1594, 1488, 1375, 1166, 754, 723, 541 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.46 (s, 1H), 7.69 (dd, J = 8.4, 0.6 Hz, 1H), 7.53 (dd, J = 7.8, 1.8 Hz, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.45 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 7.11 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 6.95 (d, J = 8.4 Hz, 2H), 6.88 (t, J = 1.8 Hz, 1H), 6.18 (dd, J = 4.2, 1.8 Hz, 1H), 6.04 (dd, J = 4.2, 2.4 Hz, 1H), 3.94 (s, 3H), 2.20 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 186.1, 143.6, 137.5, 135.9, 132.5, 132.3, 131.4, 130.3, 129.6, 129.4, 127.2, 124.2, 124.0, 123.9, 108.3, 37.7, 21.5. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{19}H_{18}N_2O_3SNa$ 377.0936; Found 377.0939.

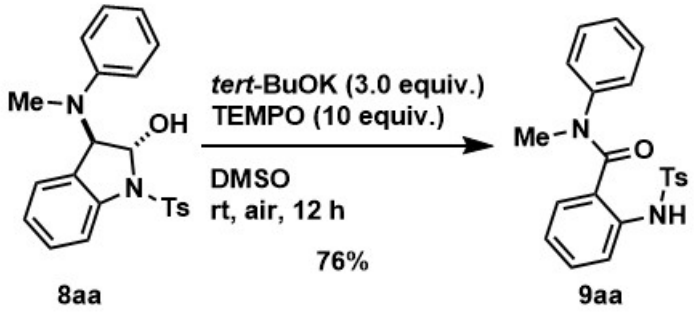


9la

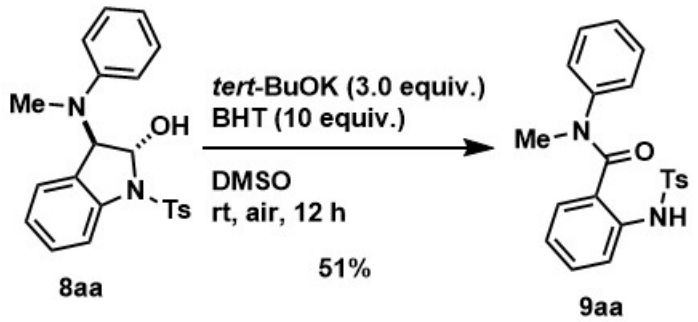
2-([1,1'-Biphenyl]-4-sulfonamido)-*N*-methyl-*N*-phenylbenzamide (9la). The reaction was performed according to the general procedure used 228 mg (0.5 mmol) of **8la**. Purification by column chromatography on silica gel using hexane/AcOEt (2/1 v/v) to give **9la**.

Pale-yellow solid (172 mg, 78% yield; mp 173–174 °C). IR (KBr) ν: 3176, 3087, 3050, 2969, 2925, 1631, 1592, 1488, 1402, 1371, 1170, 1097, 761, 701, 566 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 9.43 (br s, 1H), 7.99 (d, J = 8.4 Hz, 2H), 7.70–7.68 (m, 3H), 7.50 (d, J = 6.6 Hz, 2H), 7.43 (dd, J = 7.8, 7.8 Hz, 2H), 7.39 (dd, J = 7.2, 7.2 Hz. 1H), 7.19 (dd, J = 7.8, 7.8 Hz, 1H), 7.03–7.02 (m, 3H), 6.68 (d, J = 6.6 Hz, 1H), 6.04 (dd, J = 7.2, 7.2 Hz ,1H), 6.45 (br s, 2H), 3.42 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 169.5, 146.2, 144.5, 139.4, 137.5, 131.04, 130.04, 130.1, 129.4, 129.2, 128.7, 128.1, 127.8, 127.4, 126.9, 126.4, 124.9, 123.1, 122.4, 38.6. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{26}H_{22}N_2O_3SNa$ 465.1249; Found 465.1254.

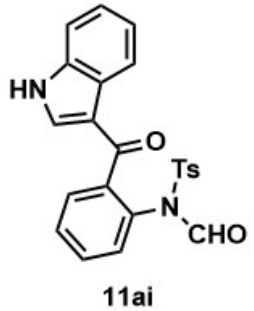
Scheme S3. Control experiments.



To a solution of **8aa** (1.0 mmol) in DMSO (5 mL, 0.2 M) were added *tert*-BuOK (337 mg, 3.0 mmol, 3.0 equiv.) and TEMPO (1.56 g, 10 mmol, 10 equiv.) under air condition. The mixture was stirred at room temperature until the complete disappearance of starting materials as indicated by TLC. After H_2O (20 mL) was added to the mixture, the whole was extracted with AcOEt (3 x 20 mL) and washed with brine (5 x 20 mL). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt (2/1 v/v) to give **9aa** (290 mg, 76%).



To a solution of **8aa** (1.0 mmol) in DMSO (5 mL, 0.2 M) were added *tert*-BuOK (337 mg, 3.0 mmol, 3.0 equiv.) and BHT (2.20 g, 10 mmol, 10 equiv.) under air condition. The mixture was stirred at room temperature until the complete disappearance of starting materials as indicated by TLC. After H_2O (20 mL) was added to the mixture, the whole was extracted with AcOEt (3 x 20 mL) and washed with brine (5 x 20 mL). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt (2/1 v/v) to give **9aa** (193 mg, 51%).

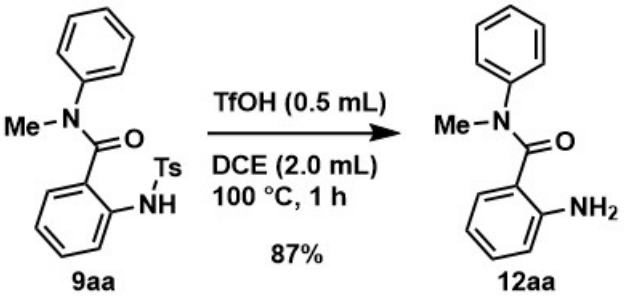


11ai

***N*-(2-(1*H*-Indole-3-carbonyl)phenyl)-*N*-tosylformamide (11ai).**

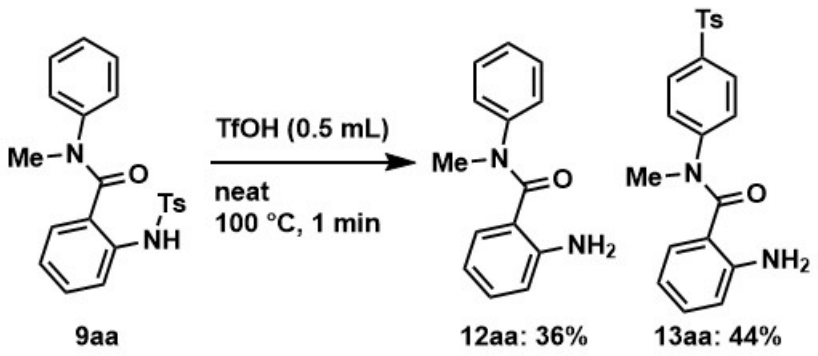
Pale-yellow solid (12.6 mg, 6% yield). IR (KBr) ν: 3342, 3185, 3056, 2923, 2852, 1610, 1436, 1340, 1159, 914, 750, 676, 565 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 12.40 (s, 1H), 10.63 (s, 1H), 8.22 (d, J = 3.0 Hz, 1H), 8.17 (d, J = 7.2 Hz, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.64 (d, J = 8.4 Hz, 2H), 7.57–7.54 (m, 2H), 7.37 (d, J = 7.8 Hz, 2H), 7.33–7.25 (m, 3H), 7.11 (d, J = 8.4 Hz, 1H), 2.36 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 197.6, 187.0, 144.6, 141.7, 136.6, 136.34, 136.34, 135.9, 134.8, 130.1, 127.5, 127.3, 125.3, 124.9, 123.8, 122.7, 122.4, 118.6, 114.3, 112.0, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{23}H_{18}N_2O_4SNa$ 441.0885; Found 441.0885.

Scheme S4. Follow up chemistry.



2-Amino-*N*-methyl-*N*-phenylbenzamide (12aa) [3c]**.** To a solution of **9aa** (38.1 mg, 0.1 mmol) in DCE (1 mL, 0.1 M) was added TfOH (0.5 mL). The mixture was stirred at 100 °C in oil bath for 1 h. After the whole was cooled to room temperature, the resulting mixture was quenched with sat. $NaHCO_3$ (5 mL) and 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 silica gel column chromatography using hexane/AcOEt (3/1 v/v) to give **12aa**.

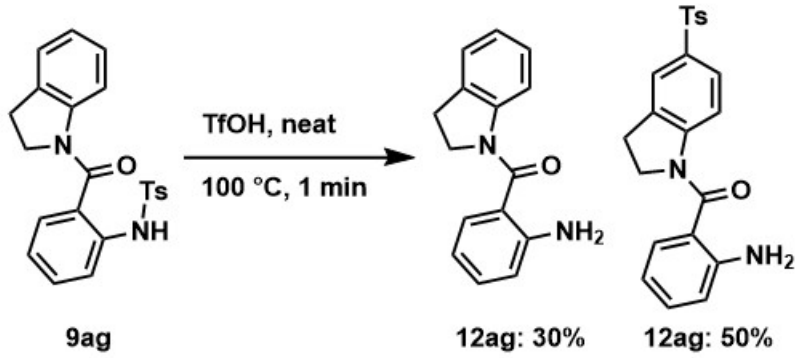
Pale-yellow oil (19.7 mg, 87% yield). IR (KBr) ν: 3434, 3367, 3062, 3035, 2925, 2854, 1619, 1585, 1492, 1371, 1159, 1027, 752, 700, 586 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.22 (dd, J = 7.8, 7.8 Hz, 2H), 7.12 (dd, J = 7.8, 7.8 Hz, 1H), 7.06 (d, J = 8.4 Hz, 2H), 6.97 (ddd, J = 8.4, 7.2, 1.2 Hz, 1H), 6.71 (dd, J = 7.8, 1.8 Hz, 1H), 6.61 (dd, J = 8.4, 1.2 Hz, 1H), 6.31 (ddd, J = 7.8, 7.8, 0.6 Hz, 1H), 4.66 (br s, 2H), 3.48 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 171.2, 147.0, 145.1, 130.6, 129.8, 129.2, 126.5, 126.4, 119.8, 116.7, 116.5, 38.1. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{14}H_{14}N_2OSNa$ 249.1004; Found 249.1004.



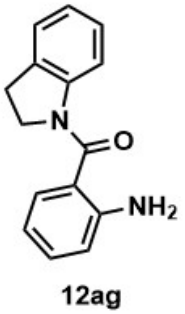
2-Amino-*N*-methyl-*N*-(4-tosylphenyl)benzamide (13aa) [3c]**. 9aa** (38.1 mg, 0.1 mmol) was stirred at 100 °C in oil bath under solvent-free condition. Then, TfOH (0.5 mL) was added to **9aa** and the mixture was stirred for

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 v/v) to give **12aa** (8.2 mg, 36%) and **13aa**.

Pale-yellow solid (16.8 mg, 44% yield; mp 162–164 °C). IR (KBr) ν: 3467, 3369, 3089, 3062, 2975, 2923, 2854, 1635, 1616, 1583, 1490, 1355, 1153, 1099, 754, 588 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.77–7.75 (m, 4H), 7.28 (d, J = 7.8 Hz, 2H), 7.15 (d, J = 8.4 Hz, 2H), 7.01 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 6.63 (dd, J = 7.8, 1.2 Hz, 2H), 6.30 (ddd, J = 7.8, 7.8, 0.6 Hz. 1H), 4.69 (br s, 2H), 3.45 (s, 3H), 2.40 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 171.4, 149.4, 147.3, 144.4, 138.9, 138.5, 131.4, 130.1, 129.7, 128.7, 127.7, 126.5, 118.5, 117.1, 116.8, 37.8, 21.7. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{21}H_{20}N_2O_3SNa$ 403.1092; Found 403.1097.



9ag (1.18 g, 3.0 mmol) was stirred at 100 °C in oil bath under solvent-free condition. Then, TfOH (1.5 mL) was added to **9ag** and the mixture was 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 (2/1 v/v) [3c].

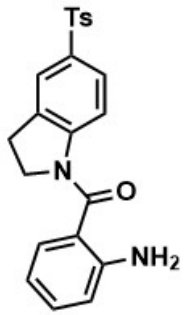


12ag

(2-Aminophenyl)(indolin-1-yl)methanone (12ag).

Pale-yellow solid (211 mg, 30% yield; 138–139 °C). IR (KBr) ν: 3469, 3372, 3031, 2954, 2894, 2859, 1635, 1579, 1479, 1400, 763 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.56 (br s, 1H), 7.25–7.20 (m, 3H), 7.13 (dd, J = 7.8, 7.8 Hz, 1H), 7.02 (dd, J = 7.2, 7.2 Hz, 1H), 6.77 (d, J = 7.8 Hz, 1H), 6.73 (dd, J = 7.2, 7.2 Hz, 1H), 4.11 (t, J = 7.8 Hz, 2H), 3.51 (br s, 2H), 3.11 (t, J = 7.2 Hz, 2H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 169.0, 145.8, 142.7, 132.8, 131.5, 128.4, 127.4, 125.1, 124.1, 122.8, 120.6, 117.7, 117.2, 50.7, 28.3. HRMS (ESI) *m/z*:

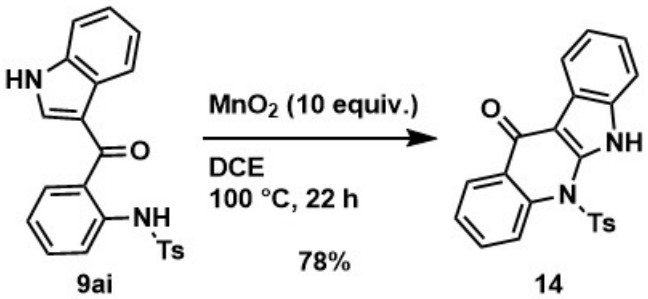
[M+Na]$^+$ Calcd for $C_{15}H_{14}N_2ONa$ 261.1004; Found 261.1008.



13ag

(2-Aminophenyl)(5-tosylindolin-1-yl)methanone (13ag).

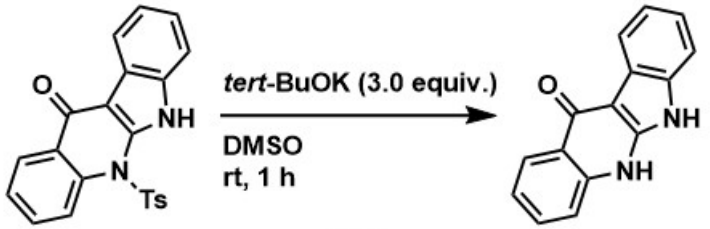
Brown oil (590 mg, 50% yield). IR (KBr) ν: 3467, 3367, 3062, 3025, 2958, 2921, 2854, 1619, 1585, 1479, 1375, 1145, 1087, 754, 661, 584 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, J = 7.8 Hz, 2H), 7.68 (s, 1H), 7.66 (d, J = 9.0 Hz, 1H), 7.63 (d, J = 8.4 Hz, 1H), 7.23 (d, J = 7.8 Hz, 2H), 7.144 (dd, J = 7.8, 7.8 Hz, 1H), 7.138 (d, J = 7.2 Hz, 1H), 6.69 (d, J = 7.8 Hz, 1H), 6.64 (dd, J = 7.8, 7.8 Hz, 1H), 4.56 (br s, 2H), 4.05 (t, J = 8.4 Hz, 2H), 3.04 (t, J = 8.4 Hz, 2H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 169.6, 146.9, 146.2, 143.8, 138.9, 136.2, 134.0, 131.8, 129.8, 128.0, 127.6, 127.2, 124.0, 118.8, 117.1, 116.9, 116.8, 50.8, 27.5, 21.4. HRMS (ESI) *m/z*: [M+Na]$^+$ Calcd for $C_{22}H_{20}N_2O_3SNa$ 415.1092; Found 415.1094.



9ai 14

5-Tosyl-5,6-dihydro-11*H*-indolo[2,3-*b*]quinolin-11-one (14) [4]**.** To a solution of **9ai** (195 mg, 0.5 mmol) in DCE (5 mL, 0.1 M) was added MnO_2 (435 mg, 10 equiv., 5 mmol). The mixture was stirred at 100 °C in oil bath for 22 h. After the whole was cooled to room temperature, the mixture was filtered with celite pad and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using hexane/AcOEt (2/1 v/v) to give **14**.

Pale-yellow solid (152 mg, 78% yield; 178–180 °C). IR (KBr) ν: 3156, 3089, 2884, 1623, 1596, 1498, 1382, 1172, 779, 667 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.05 (br s, 1H), 8.49 (d, J = 8.4 Hz, 1H), 8.379 (d, J = 7.8 Hz, 1H), 8.376 (d, J = 7.8 Hz, 1H), 7.65 (ddd, J = 9.0, 7.2, 1.8 Hz, 1H), 7.55 (d, J = 7.8 Hz, 1H), 7.48 (dd, J = 7.8, 7.8 Hz, 1H), 7.39 (dd, J = 7.2, 7.2 Hz, 1H), 7.35 (dd, J = 7.8, 7.8 Hz, 1H), 7.23 (d, J = 8.4 Hz, 2H), 7.00 (d, J = 7.8 Hz, 2H), 2.24 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 175.0, 146.5, 141.6, 136.9, 133.6, 132.1, 131.6, 130.1, 128.0, 126.95, 126.85, 126.6, 124.7, 123.0, 122.7, 122.1, 121.9, 111.3, 107.0, 21.7. HRMS (ESI) *m/z*: [M+Na]$^+$ Calcd for $C_{22}H_{16}N_2O_3SNa$ 411.0779; Found 411.0779.



14 4

5*H*,6*H*-Quinindolin-11-one (4) [1a, 6]**.** To a solution of **14** (116.5 mg, 0.3 mmol) in DMSO (1.5 mL, 0.2 M) was added *t*BuOK (101 mg, 3.0 equiv., 0.9 mmol). The mixture was stirred at room temperature for 1 h. After the mixture was quenched with H_2O (10 mL), the whole was extracted with AcOEt (3 x 10 mL) and washed with brine (10 mL). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by silica gel column chromatography using $CHCl_3$/MeOH (6/1 v/v) to give **4**.

Pale-yellow solid (41 mg, 58% yield; mp > 300 °C). IR (KBr) ν: 3274, 3095, 3048, 2965, 1617, 1411, 1197, 740 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 12.16 (br s, 1H), 11.53 (br s, 1H), 8.29 (d, J = 7.8 Hz, 1H), 8.18 (d, J = 7.2 Hz, 1H), 7.64–7.63 (m. 2H), 7.47 (d, J = 7.8 Hz, 1H), 7.31–7.29 (m, 1H), 7.24 (dd, J = 7.8, 7.8 Hz, 1H), 7.19 (dd, J = 7.2, 7.2 Hz, 1H); $^{13}C\{^1H\}$ NMR (151 MHz, DMSO-d_6) δ 172.3, 145.3, 138.3, 135.0, 130.8, 125.3, 123.8, 123.6, 122.7, 121.5, 120.9, 120.0, 117.5, 110.9, 101.8. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{15}H_{10}N_2ONa$ 257.0691; Found 257.0694.

9aq 15

***trans*-6-Hydroxy-5-tosyl-5a,6-dihydroindolo[2,1-*b*]quinazolin-12(5*H*)-one (15)** [7]**. 9aq** (39.0 mg, 0.1 mmol), iodobenzene diacetate (48.3 mg, 1.5 equiv., 0.15 mmol) and eosin-Y (2.1 mg, 3.0 mol%) in MeCN (2 mL) was stirred at room temperature under the irradiation of 8 W blue LED (448 nm) for 2 h. After H_2O (5 mL) was added to the mixture, the whole was 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 (3/1 v/v) to give **8la**.

Pale-yellow solid (16.9 mg, 42% yield). IR (KBr) ν: 3361, 3064, 3048, 3029, 2960, 2927, 1644, 1484, 1427, 1359, 1168, 763, 674 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ 7.98 (d, J = 7.8 Hz, 1H), 7.82 (d, J = 7.8 Hz, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.67 (dd, J = 8.4, 8.4 Hz, 1H), 7.51 (d, J = 8.4 Hz. 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.29 (dd, J = 7.8, 7.8 Hz, 1H), 7.19 (dd, J = 7.2, 7.2 Hz, 1H), 6.86–6.83 (m, 5H), 5.50 (d, J = 4.8 Hz, 1H), 2.78 (br s, 1H), 2.25 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 159.2, 145.0, 140.5, 140.4, 134.2, 133.1, 130.3, 130.1,

129.5, 128.4, 128.2, 127.3, 127.0, 125.6, 125.2, 115.3, 84.4, 71.8, 21.6. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{22}H_{18}N_2O_4SNa$ 429.0885; Found 429.0887.

Reference

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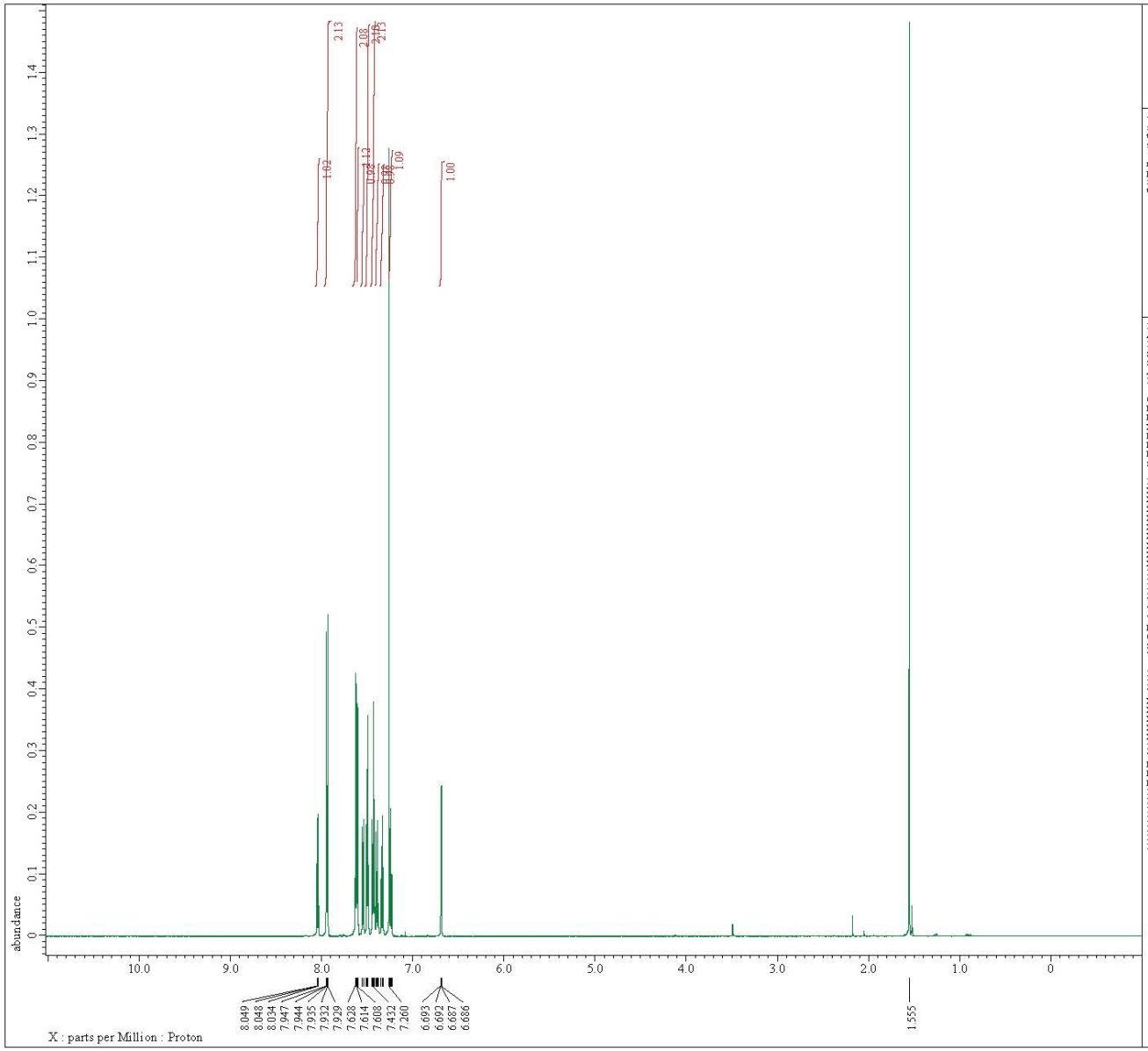

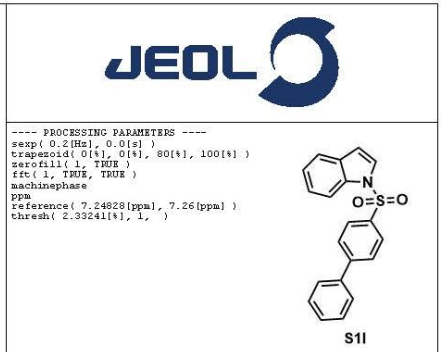

S1l

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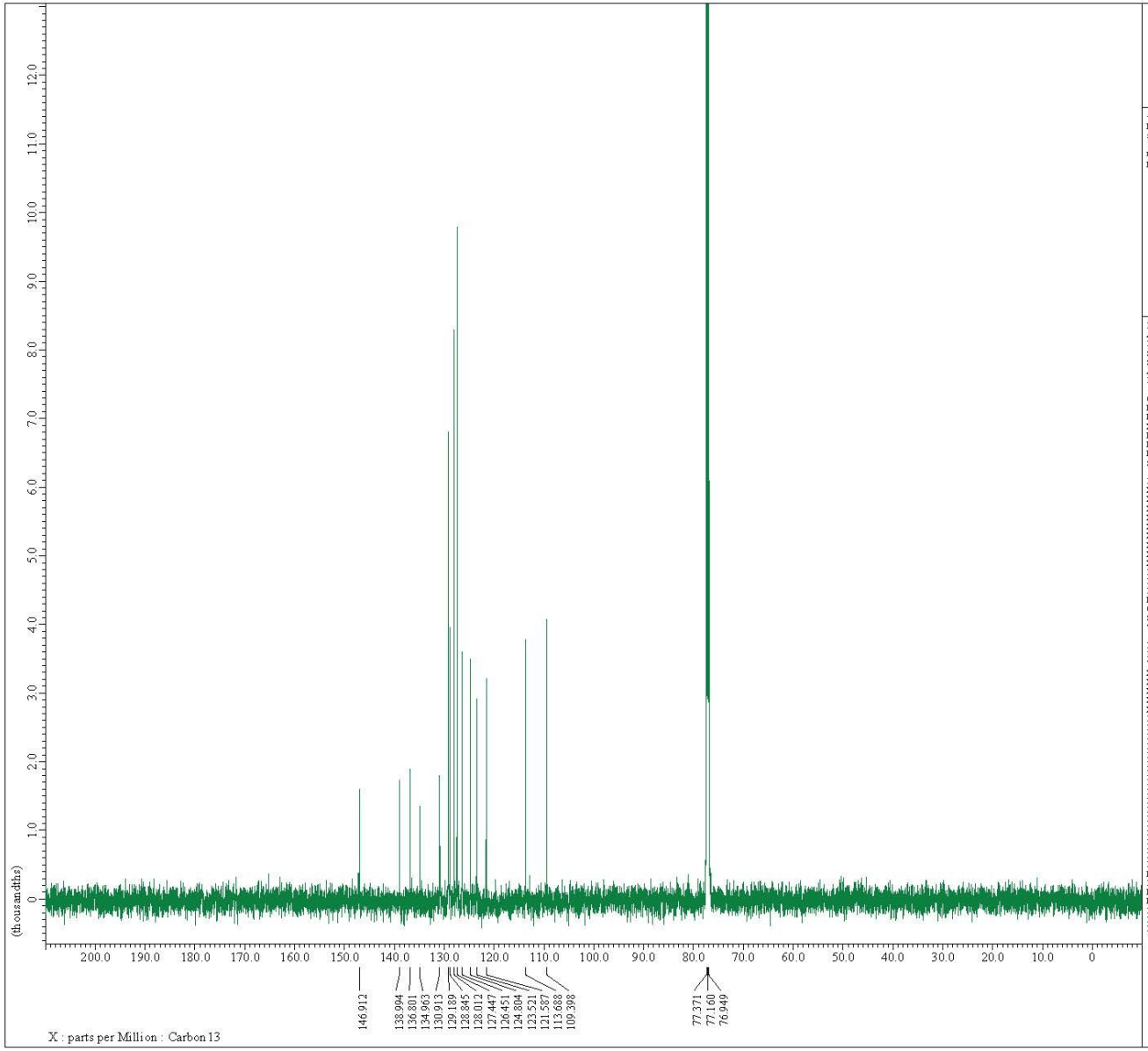

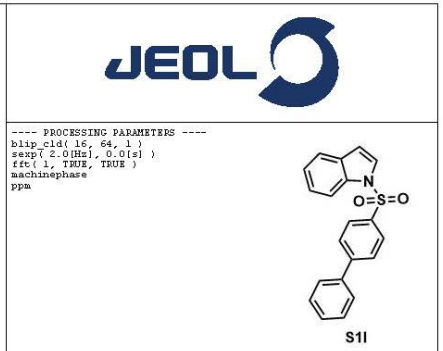


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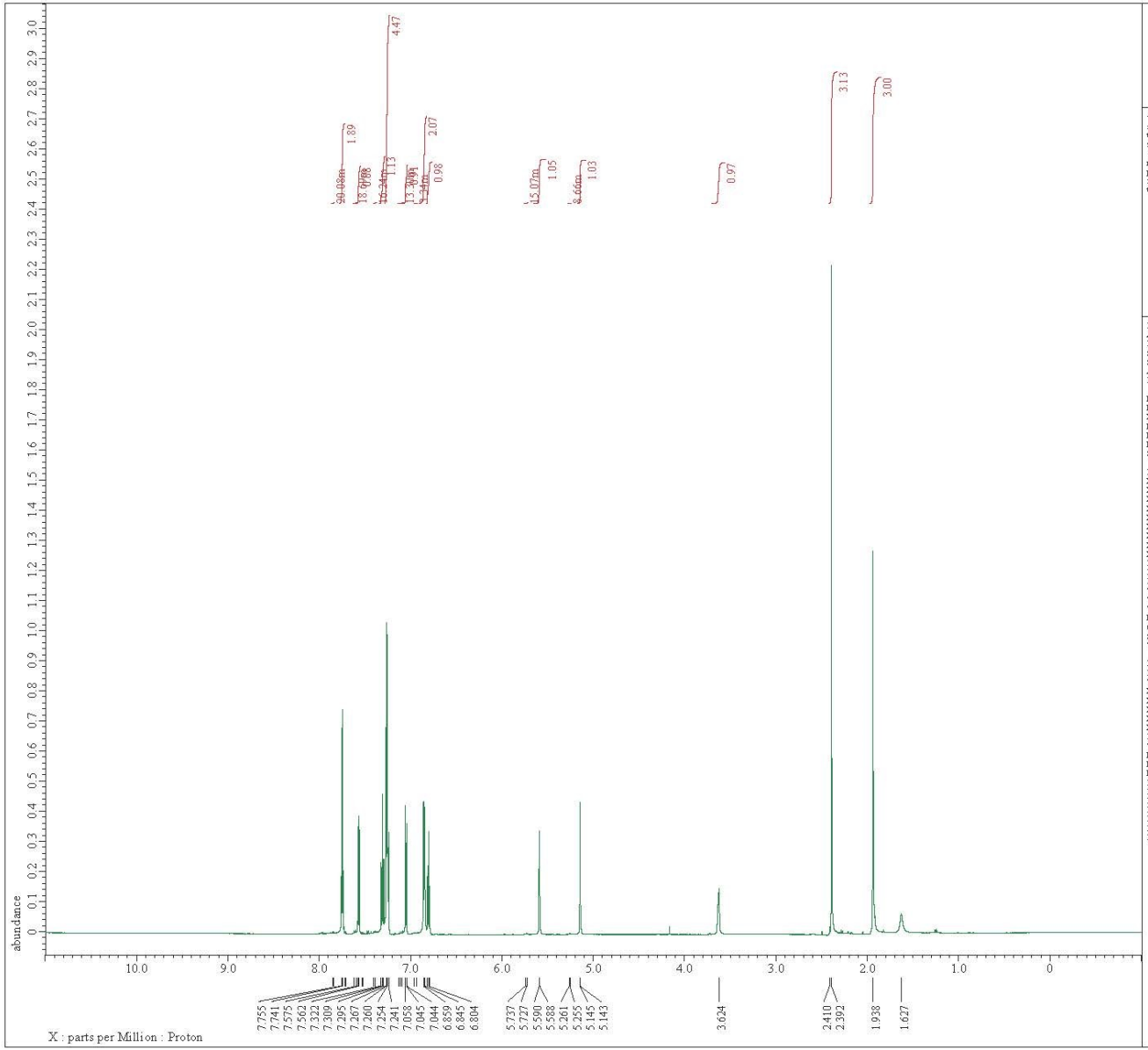
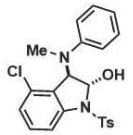
S1l

```
Filename                    = TK-6-052-1_carbon-1-3.jdf
Author                      = delta
Experiment                  = carbon.jxp
Sample_Id                   = TK-6-052-1
Solvent                     = CHLOROFORM-D
Actual_Start_Time           = 22-MAR-2024 20:41:13
Revision_Time               =  2-JUL-2024 19:39:41

Comment                     = single pulse decoupled gated NOE
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                    = 20.3[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_Factor        = 2.2
Irr_Decoupling              = TRUE
Irr_Noe                     = TRUE
Irr_Noise                   = WALTZ
Irr_Offset_Default          = 5[ppm]
Irr_Pwidth                  = 76[us]
Irr_Pwidth_Default          = 76[us]
Irr_Pwidth_Default_Calc     = 76[us]
Irr_Pwidth_Templ            = 76[us]
Irr_Wurst                   = FALSE
Decimation_Rate             = 0
Initial_Wait                = 1[s]
Noe_Time                    = 2[s]
Noe_Time_Flag               = FALSE
Relaxation_Delay_Calc       = 0[s]
Relaxation_Delay_Temp       = 2[s]
Repetition_Time             = 2.69206016[s]
```

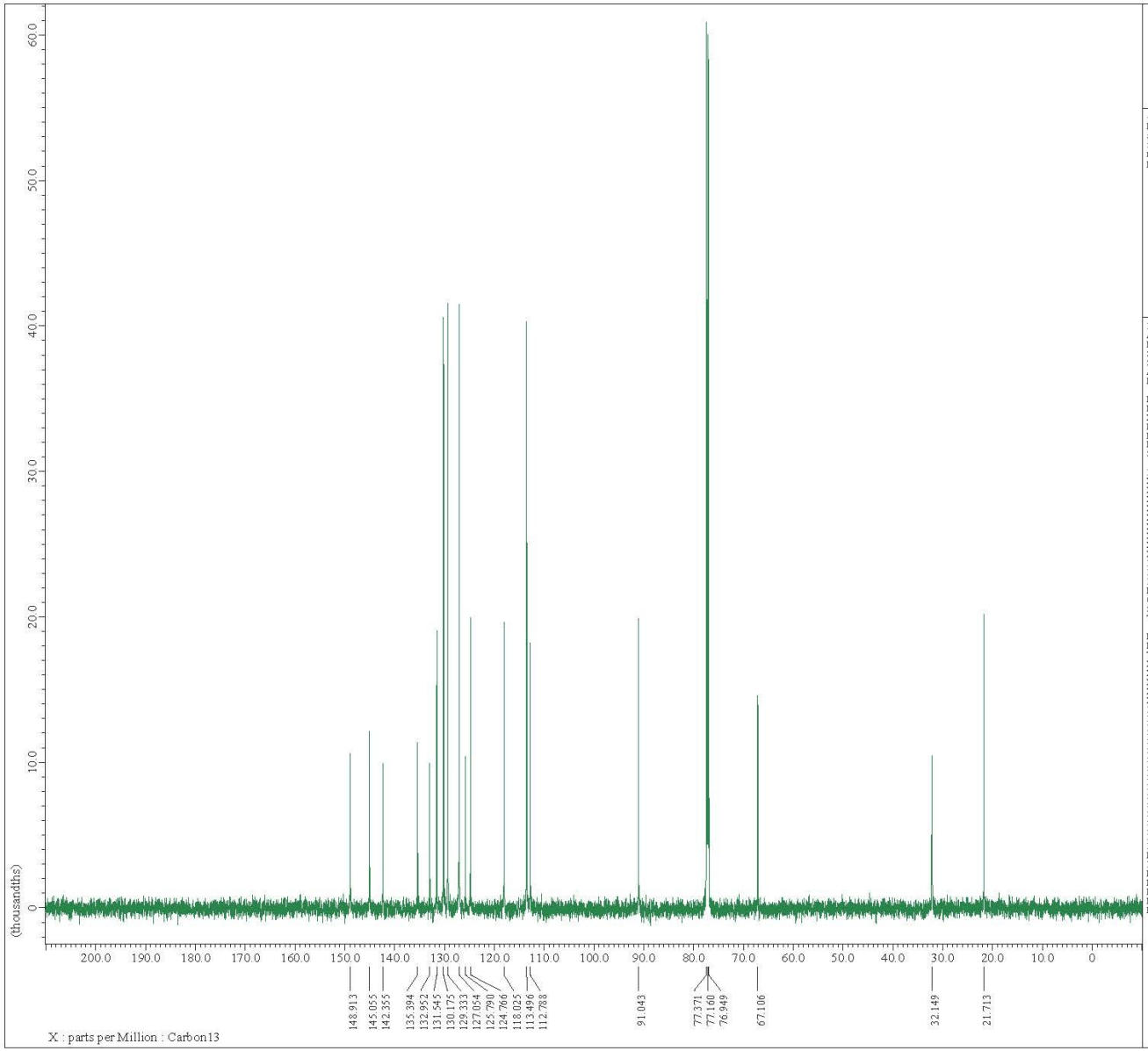


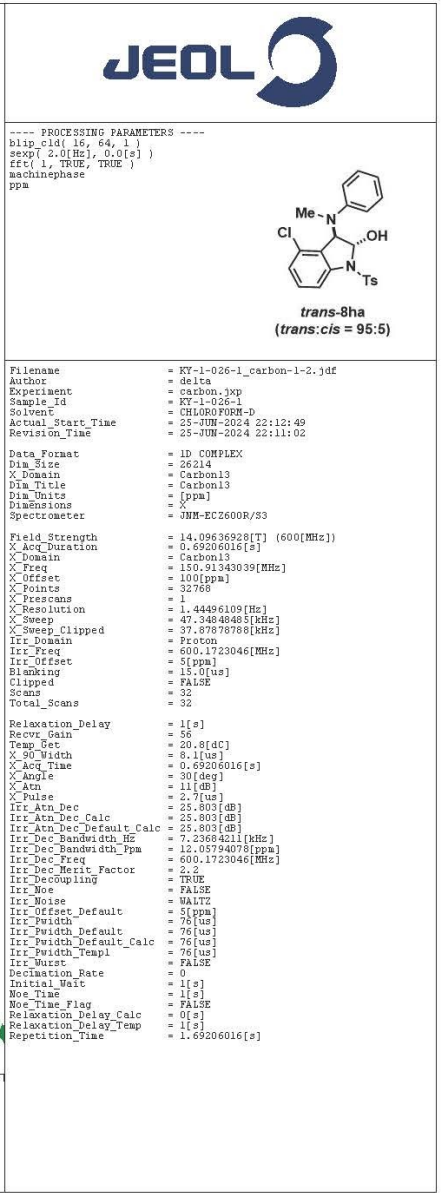

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.24764[ppm], 7.26[ppm] )
thresh( 2.67219[%], 1, )
```



***trans*-8ha**
(*trans*:*cis* = 95:5)

```
Filename                = KY-1-026-1-2_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = KY-1-026-1-2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 26-JUN-2024 22:10:30
Revision_Time           =  5-AUG-2024 11:15:01

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          = 2.91110912[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 32768
X_Prescans              = 1
X_Resolution            = 0.34351169[Hz]
X_Sweep                 = 11.2561909[kHz]
X_Sweep_Clipped         = 9.00496272[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              = 46
Temp_Get                = 21.1[dC]
X_90_Width              = 9.9[us]
X_Acq_Time              = 2.91110912[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                   = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.91110912[s]
```

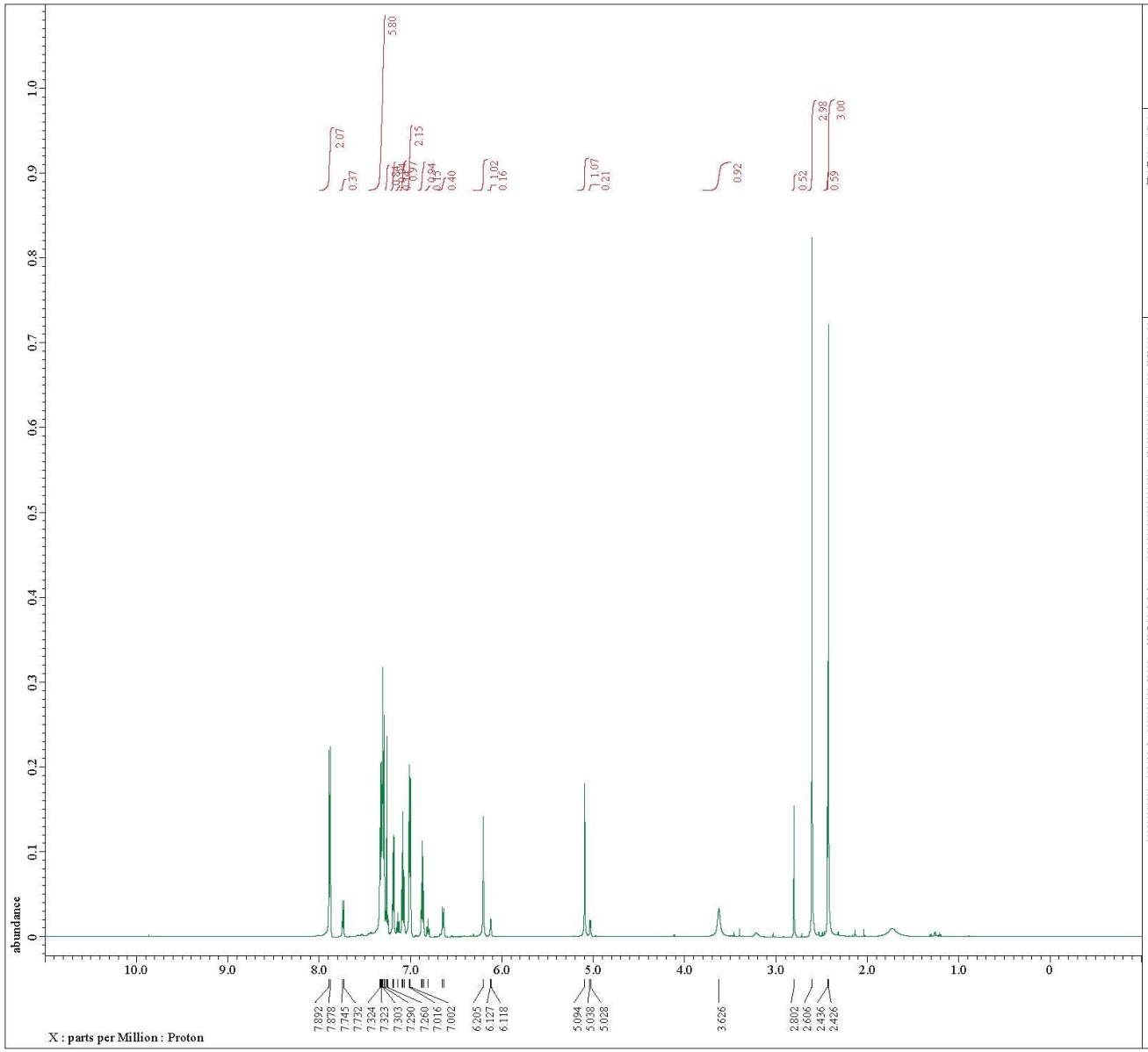





```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

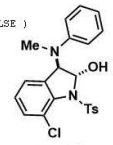

***trans*-8ha**
(***trans*:*cis*** = 95:5)

```
Filename                    = KY-1-026-1_carbon-1-2.jdf
Author                      = delta
Experiment                  = carbon.jxp
Sample_Id                   = KY-1-026-1
Solvent                     = CHLOROFORM-D
Actual_Start_Time           = 25-JUN-2024 22:12:49
Revision_Time               = 25-JUN-2024 22:11:02

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                       = 32
Total_Scans                 = 32

Relaxation_Delay            = 1[s]
Recvr_Gain                  = 56
Temp_Set                    = 20.8[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_Dec_Bandwidth_Hz        = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm       = 12.05794078[ppm]
Irr_Dec_Freq                = 600.1723046[MHz]
Irr_Dec_Merit_Factor        = 2.2
Irr_DecCupling              = TRUE
Irr_Noe                     = FALSE
Irr_Noise                   = WALTZ
Irr_Offset_Default          = 5[ppm]
Irr_Pwidth                  = 76[us]
Irr_Pwidth_Default          = 76[us]
Irr_Pwidth_Default_Calc     = 76[us]
Irr_Pwidth_Temp1            = 76[us]
Irr_Wurst                   = FALSE
Declination_Rate            = 0
Initial_Wait                = 1[s]
Noe_Time                    = 1[s]
Noe_Time_Flag               = FALSE
Relaxation_Delay_Calc       = 0[s]
Relaxation_Delay_Temp       = 1[s]
Repetition_Time             = 1.69206016[s]
```



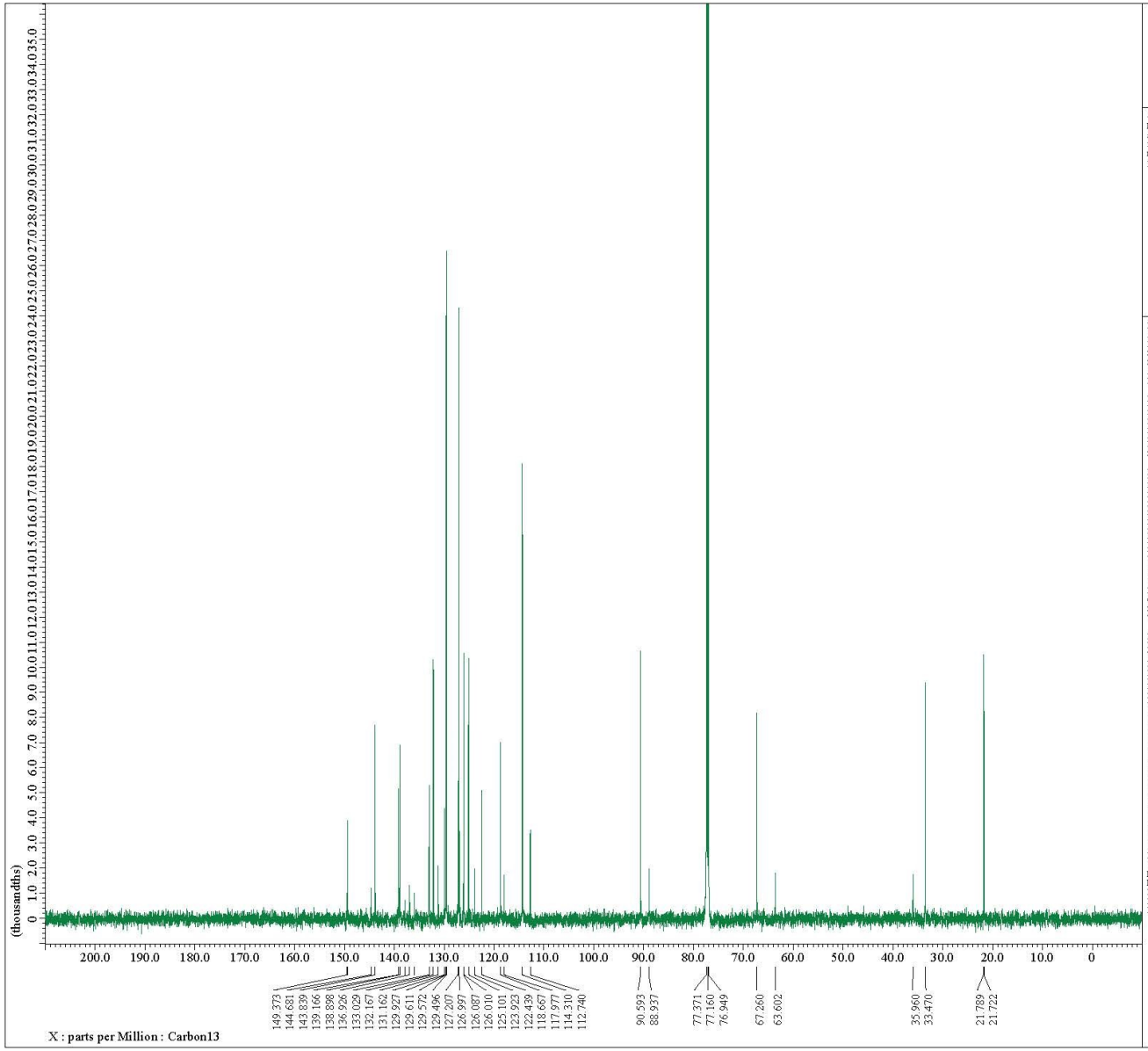
JEOL

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



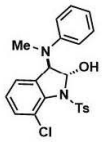
***trans*-8ja**
(***trans*:*cis*** = 85:15)

```
Filename                = TK-6-151-0-2_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-151-0-2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 26-JUN-2024 22:23:46
Revision_Time           = 27-JUN-2024 08:16:55

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[MHz])
X_Acq_Duration          = 2.91110912[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 32768
X_Prescans              = 1
X_Resolution            = 0.34351169[Hz]
X_Sweep                 = 11.2561909[kHz]
X_Sweep_Clipped         = 9.00495272[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_Get                = 20.9[dC]
X_90_Width              = 9.9[us]
X_Acq_Time              = 2.91110912[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                   = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.91110912[s]
```



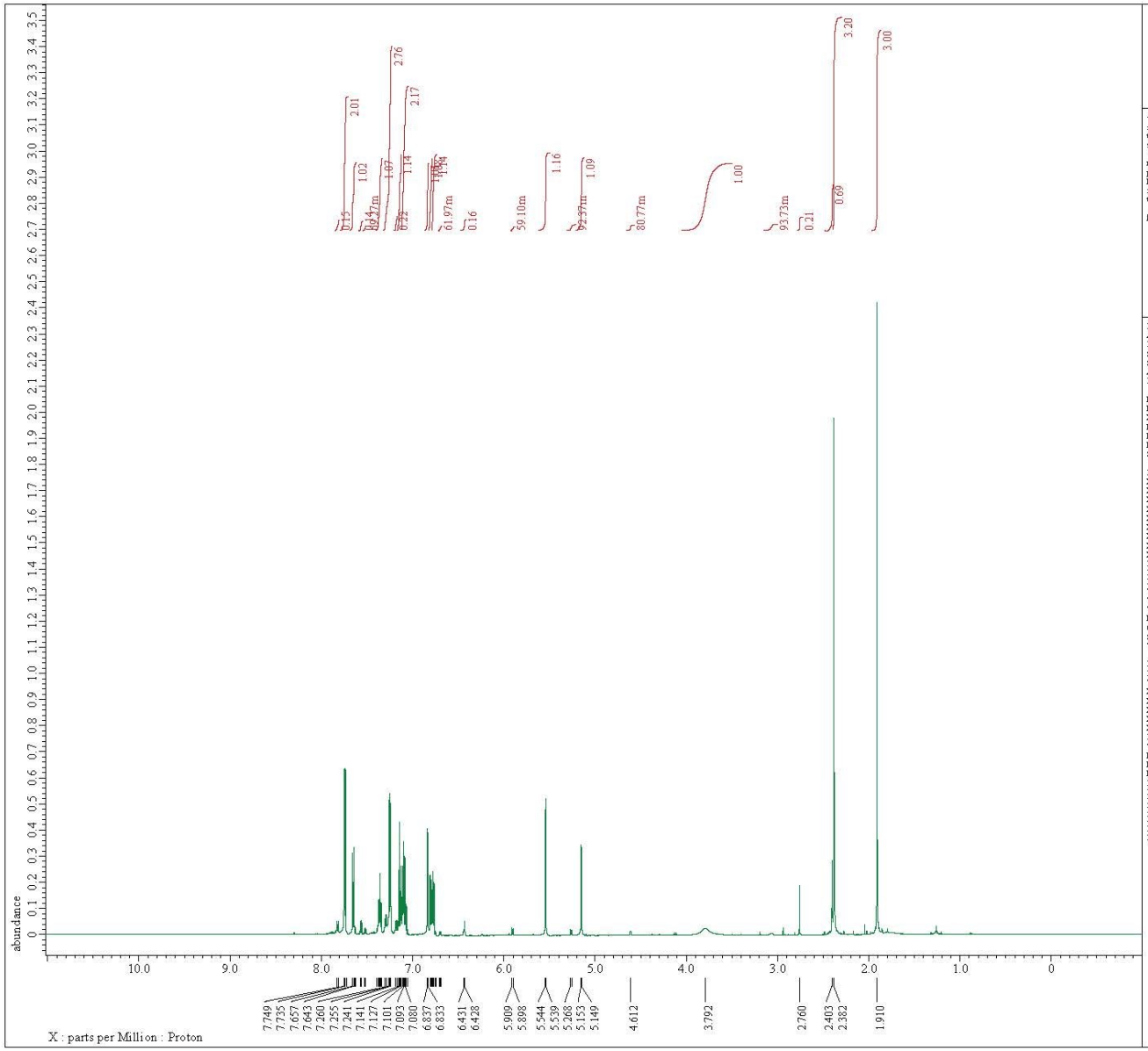
JEOL

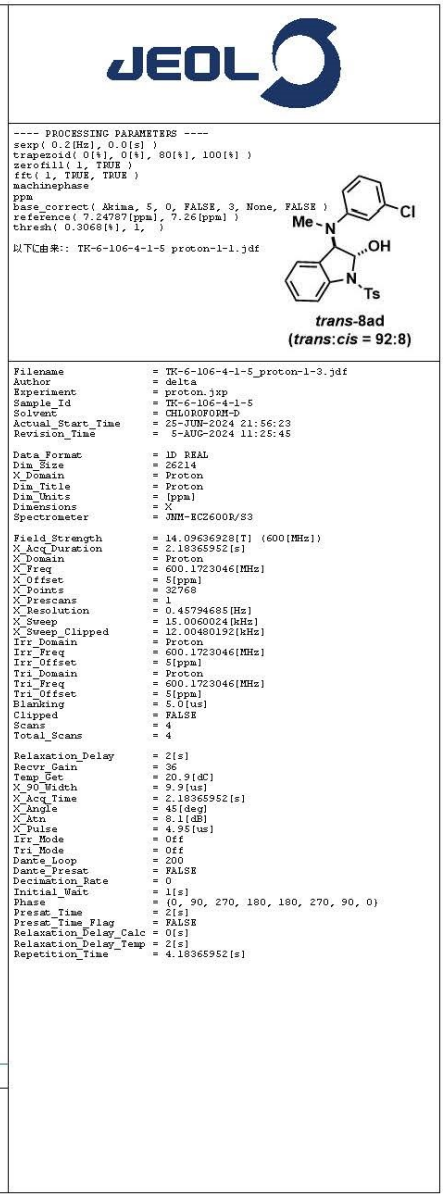
```
---- PROCESSING PARAMETERS ----
blip_cid( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```



***trans*-8ja**
(***trans*:*cis*** = 85:15)

Filename	= TK-6-151-0-2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-151-0-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-JUN-2024 22:25:56
Revision_Time	= 26-JUN-2024 22:52:26
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	= 128
Total_Scans	= 128
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

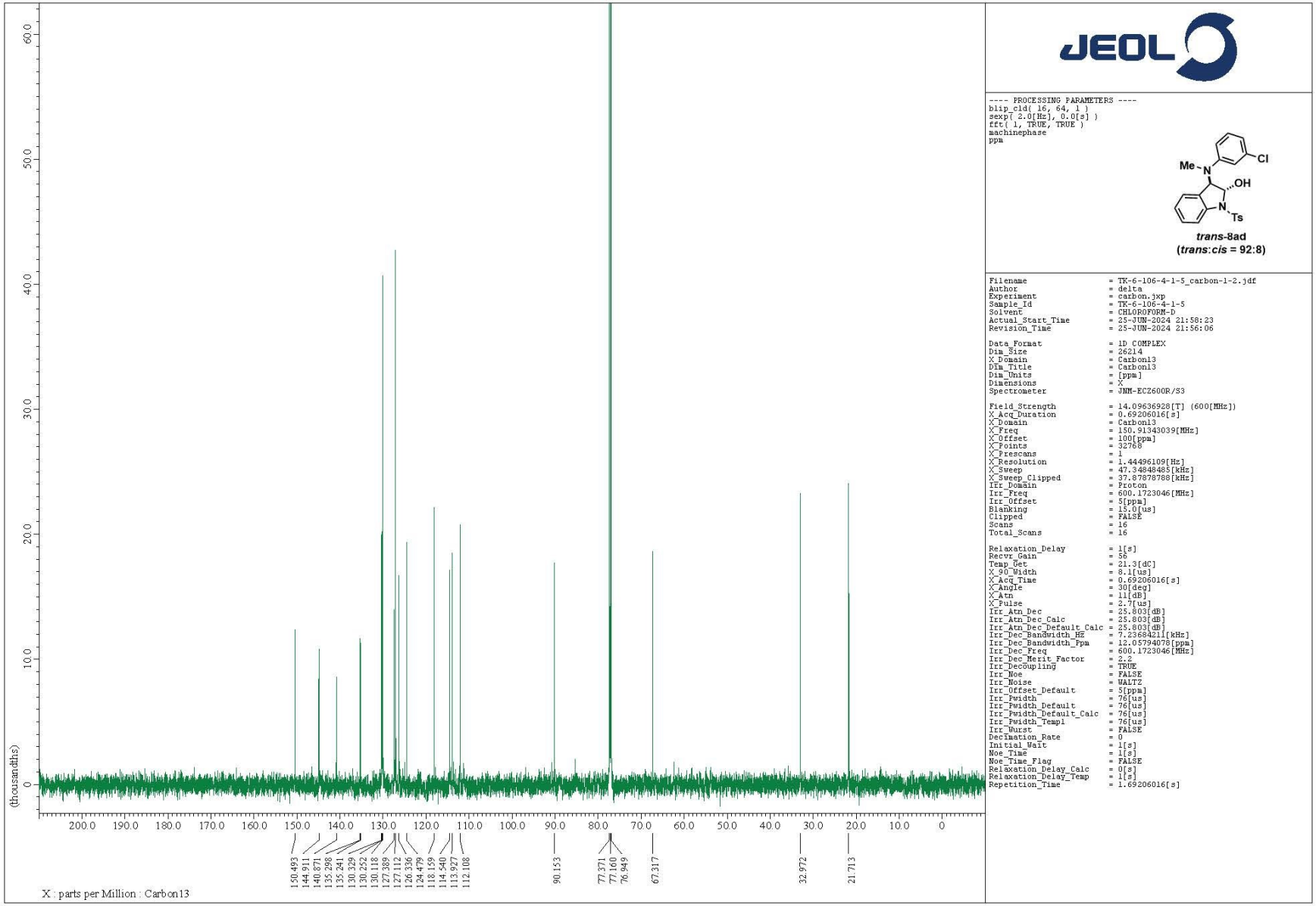


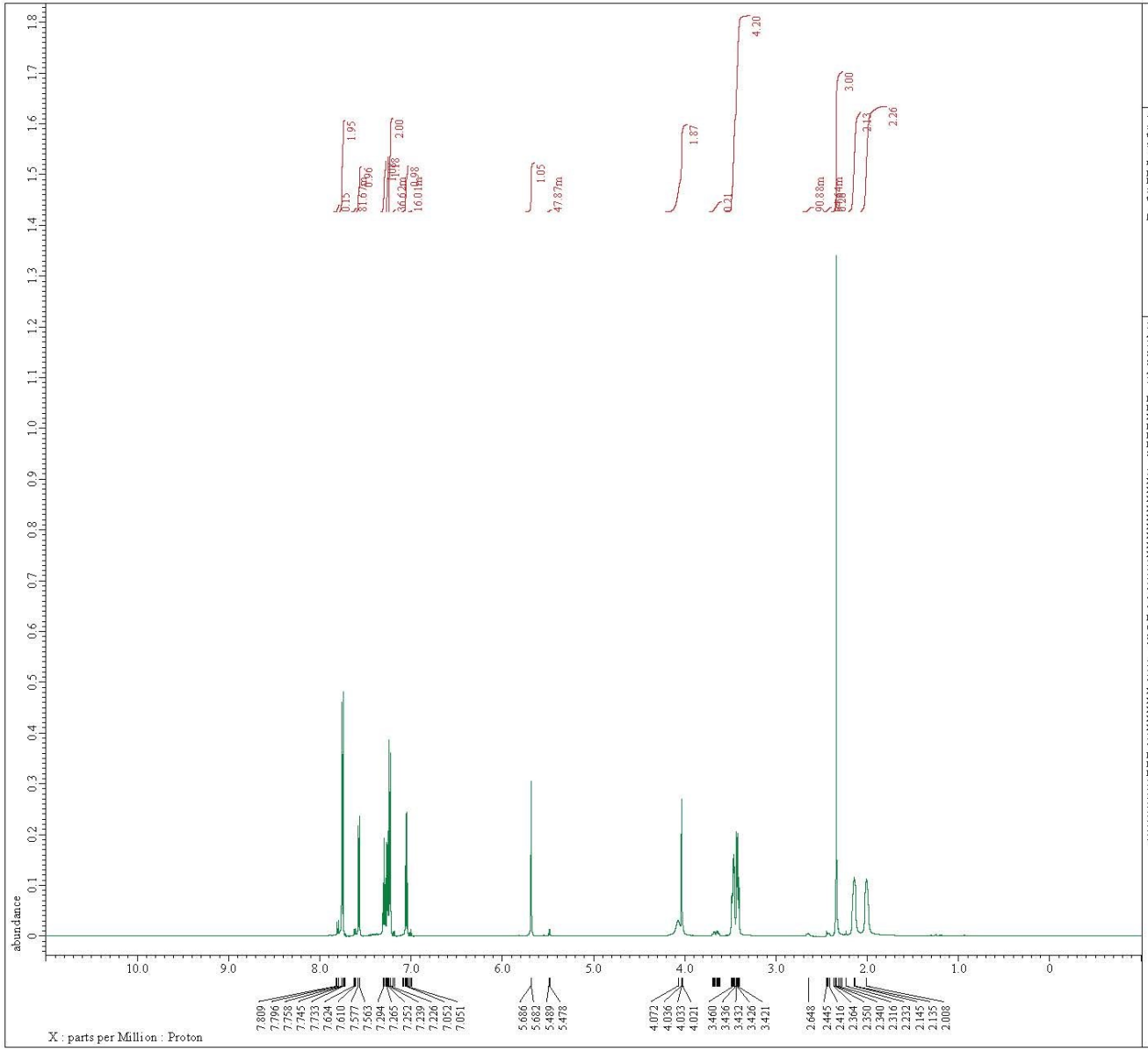


```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FALSE )
reference( 7.24787[ppm], 7.26[ppm] )
thresh( 0.3068[%], 1, )

以下由来:: TK-6-106-4-1-5 proton-1-1.jdf
```


***trans*-8ad**
(***trans*:*cis*** = 92:8)

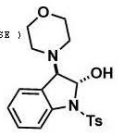
```
Filename              = TK-6-106-4-1-5_proton-1-3.jdf
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TK-6-106-4-1-5
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-JUN-2024 21:56:23
Revision_Time         =  5-AUG-2024 11:25:45

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[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            = 36
Temp_Get              = 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                 = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time           = 2[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time       = 4.18365952[s]
```


(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
150.493
144.911
140.671
135.298
135.241
130.329
130.252
130.118
127.389
127.112
126.336
124.479
118.159
114.540
113.927
112.108
90.153
77.371
77.160
76.949
67.317
32.972
21.713
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
Me
N
Cl
OH
N
Ts
trans-8ad
(trans:cis = 92:8)
Filename = TK-6-106-4-1-5_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-106-4-1-5
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-JUN-2024 21:58:23
Revision_Time = 25-JUN-2024 21:56:06
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 = 16
Total_Scans = 16
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 21.3[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_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_DecCupling = TRUE
Irr_Noe = FALSE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Unst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]



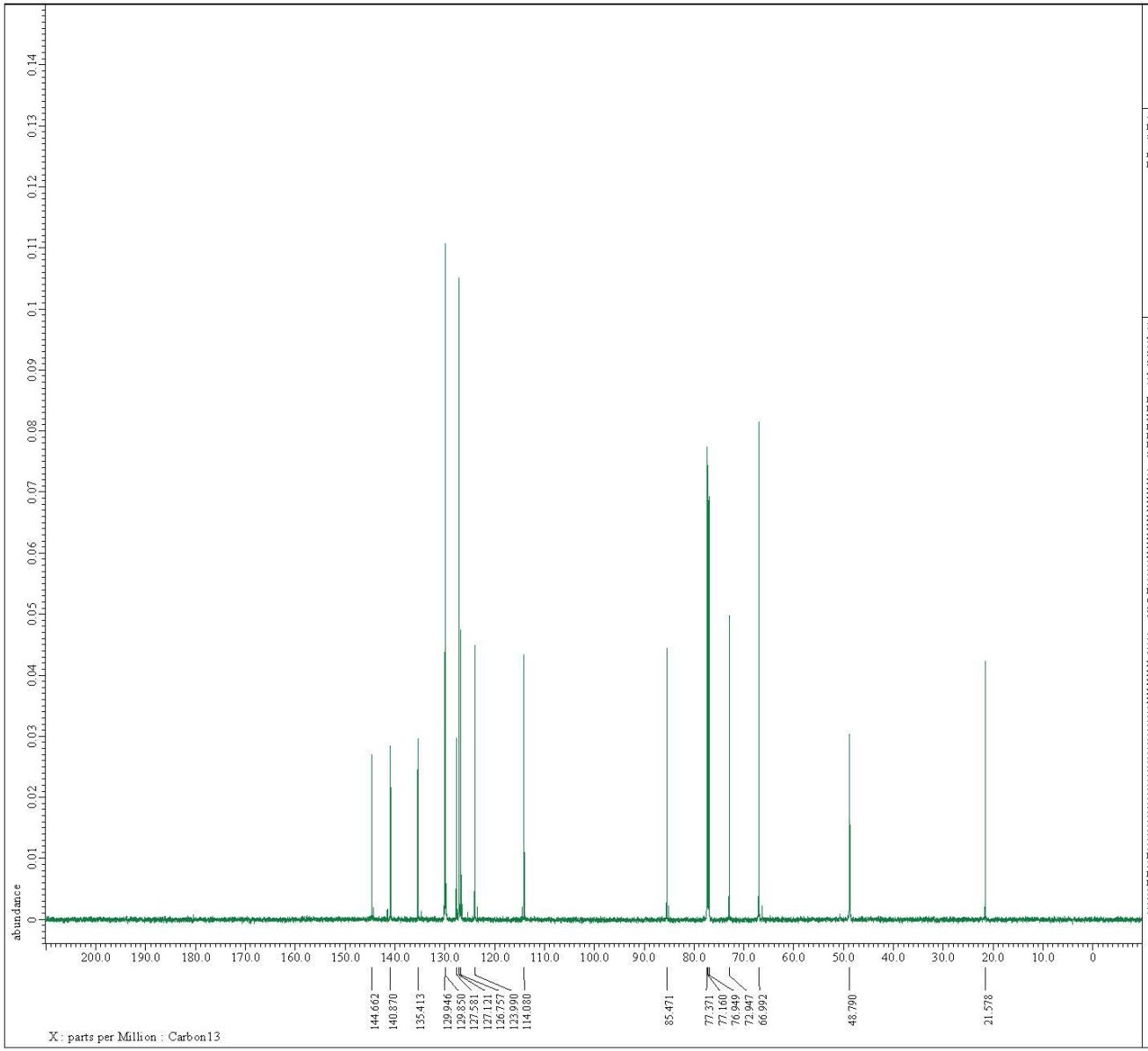
JEOL

```
---- 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, FALSE )
reference( 7.24787[ppm], 7.26[ppm] )
thresh( 0.25655[%], 1, )

以下由来:: TK-6-300-1 proton-1-1.jdf
```



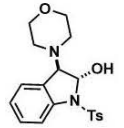
***trans*-8af**
(***trans*:*cis*** = 92:8)

```
Filename                = TK-6-300-1_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-300-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 29-JUN-2024 21:49:59
Revision_Time           =  5-AUG-2024 11:31:11

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[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_Get                = 21.3[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```



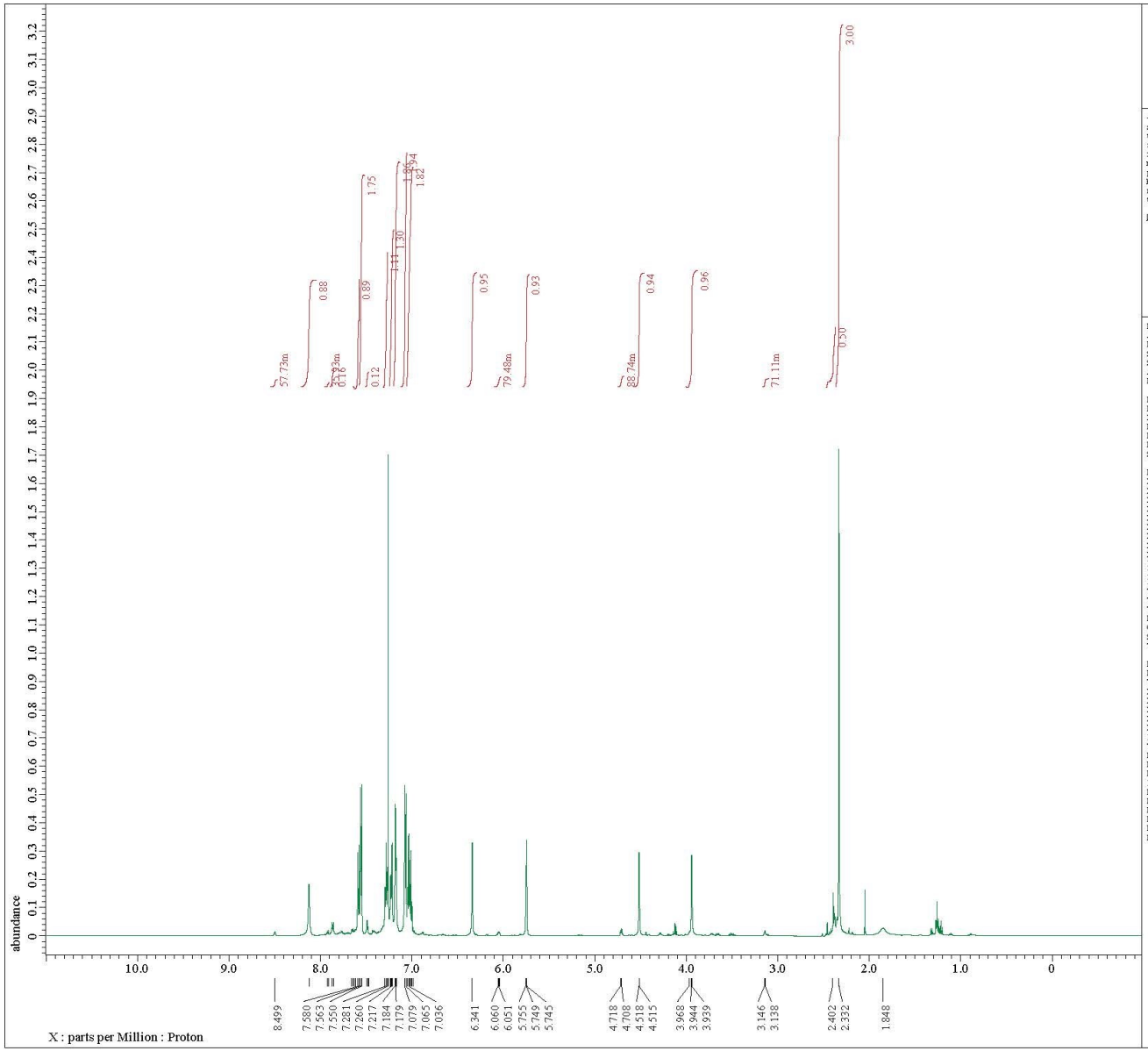
JEOL

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

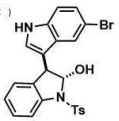


***trans*-8af**
(***trans*:*cis*** = 92:8)

Filename	= TK-6-300-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-300-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JUN-2024 21:50:48
Revision_Time	= 29-JUN-2024 21:51:09
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	= 86
Total_Scans	= 86
Relaxation_Delay	= 1[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_Dec_Bandwidth_Hz	= 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

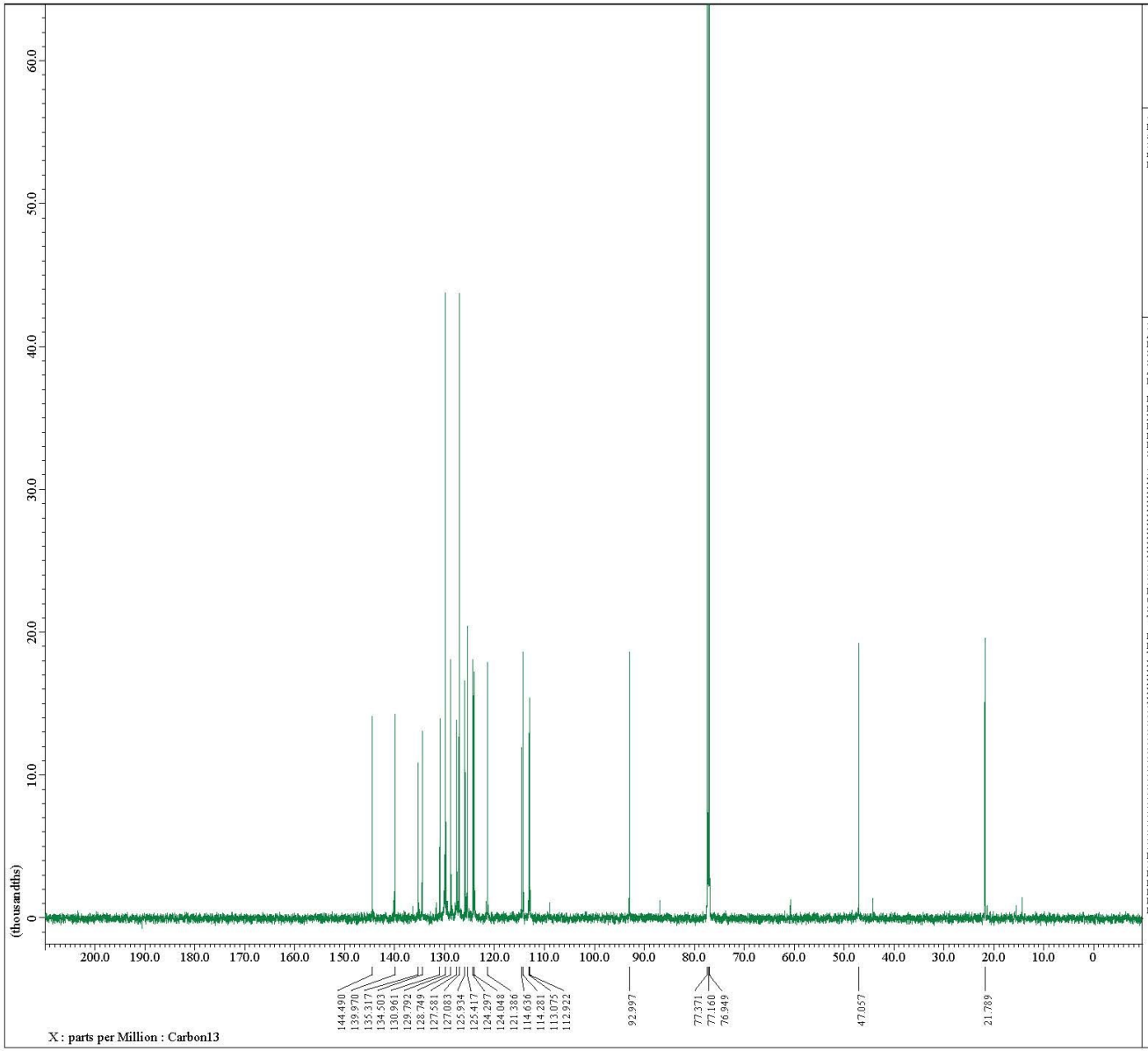



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FALSE )
reference( 7.24711[ppm], 7.26[ppm] )
thresh( 0.61274[%], 1, )

以下は由来:: TK-6-122-4-15 proton-1-1.jdf
```



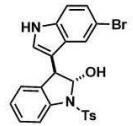
***trans*-8am**
(***trans*:*cis*** = 92:8)

```
Filename                = TK-6-122-4-15_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-122-4-15
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  1-JUL-2024 19:51:37
Revision_Time           =  5-AUG-2024 11:39:15

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[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              = 36
Temp_Get                = 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                   = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```



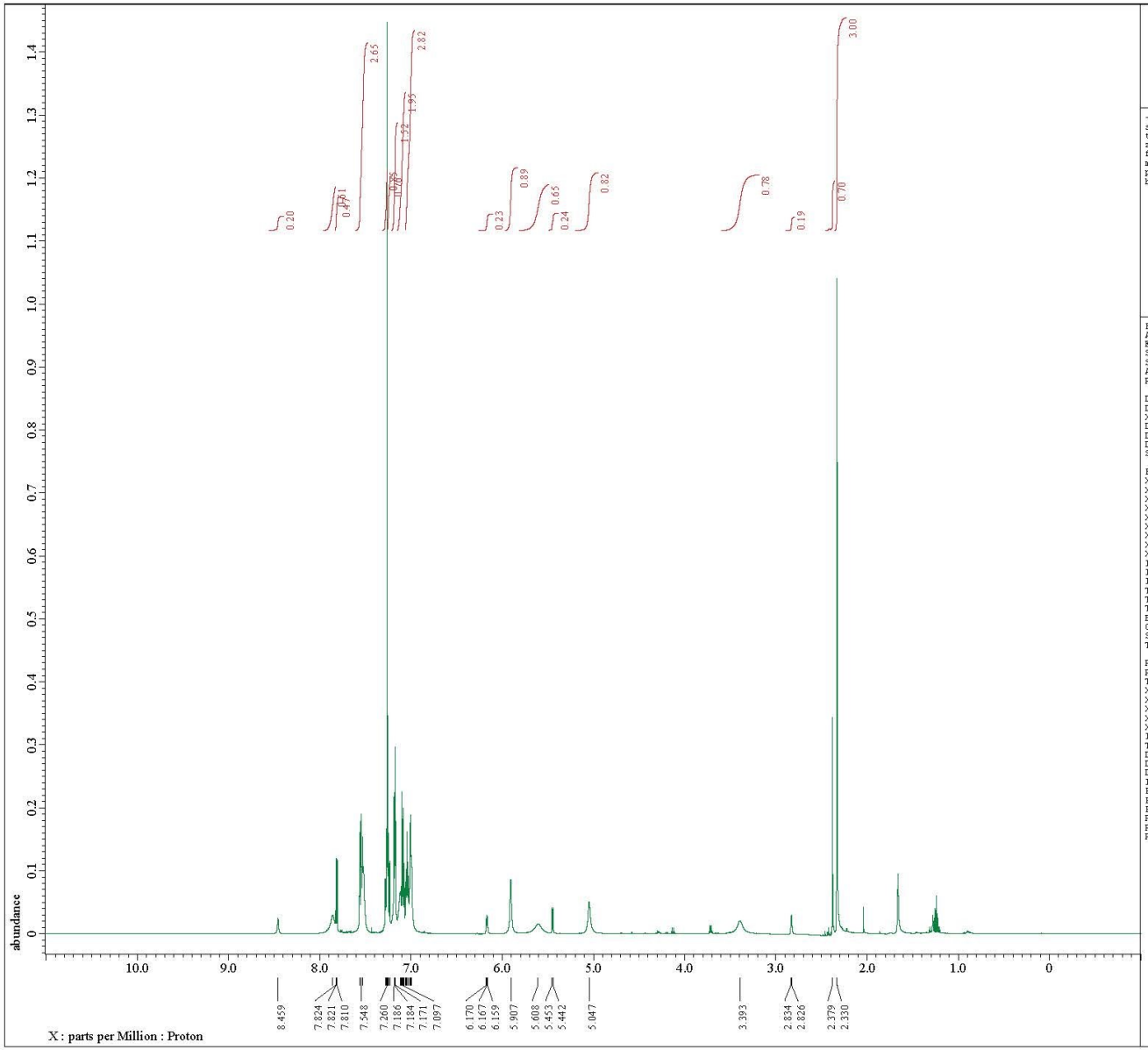
JEOL

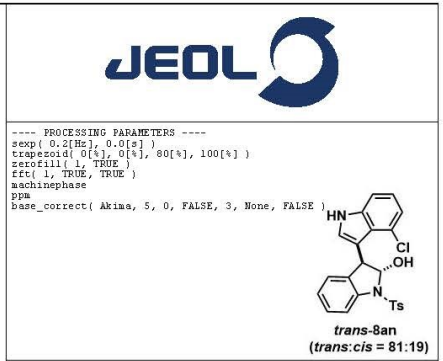
```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```



***trans*-8am**
(***trans*:*cis*** = 92:8)

```
Filename                = TK-6-122-4-15_carbon-1-2.jdf
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = TK-6-122-4-15
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  1-JUL-2024 19:52:24
Revision_Time           =  1-JUL-2024 19:54:32

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                   = 130
Total_Scans             = 130

Relaxation_Delay        = 1[s]
Recvr_Gain              = 56
Temp_Set                = 21[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_Dec_Bandwidth_Hz    = 7.236842[1][kHz]
Irr_Dec_Bandwidth_Ppm   = 12.05794078[ppm]
Irr_Dec_Freq            = 600.1723046[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = FALSE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 76[us]
Irr_Pwidth_Default      = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ        = 76[us]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Noe_Time                = 1[s]
Noe_Time_Flag           = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 1[s]
Repetition_Time         = 1.69206016[s]
```

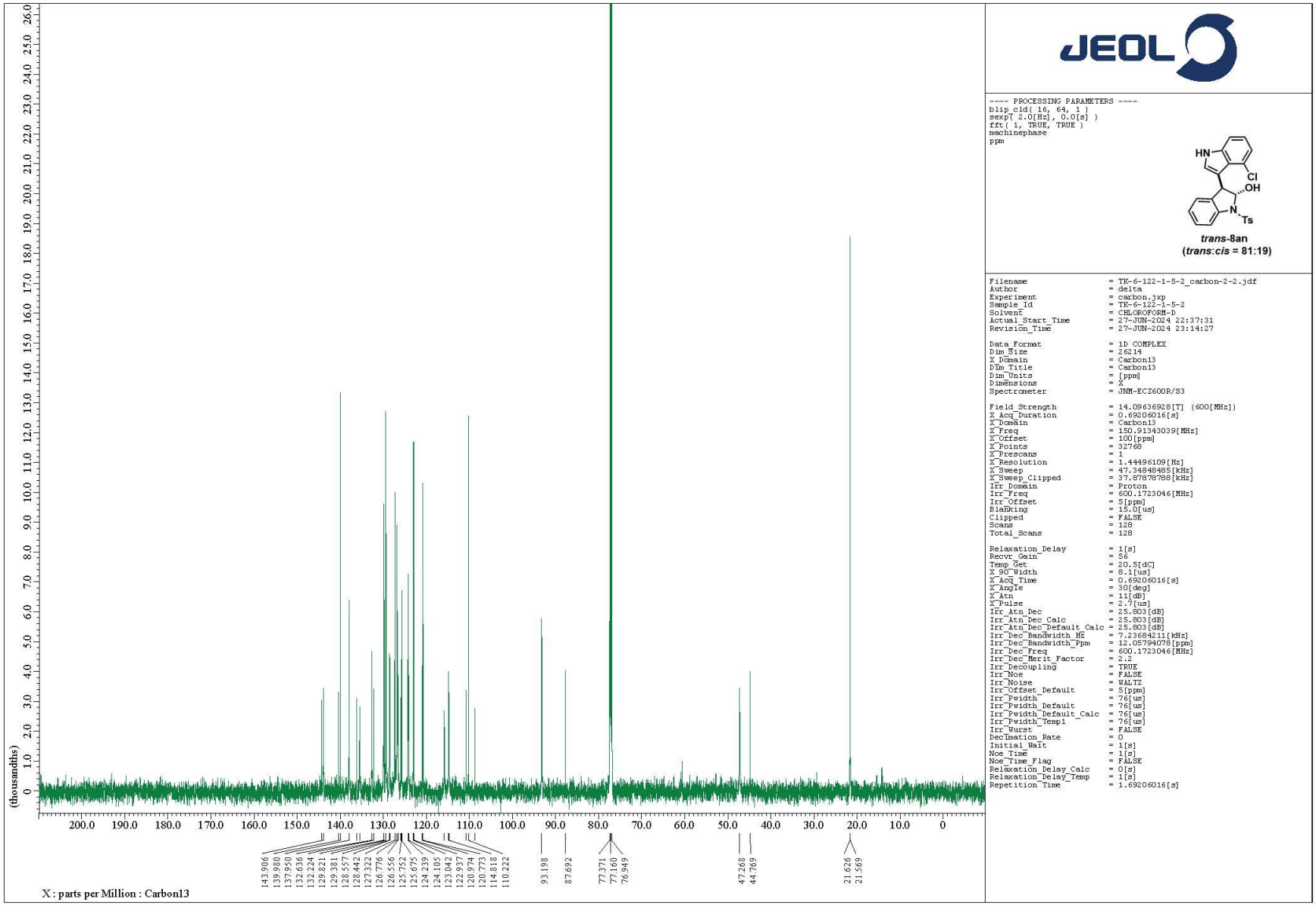


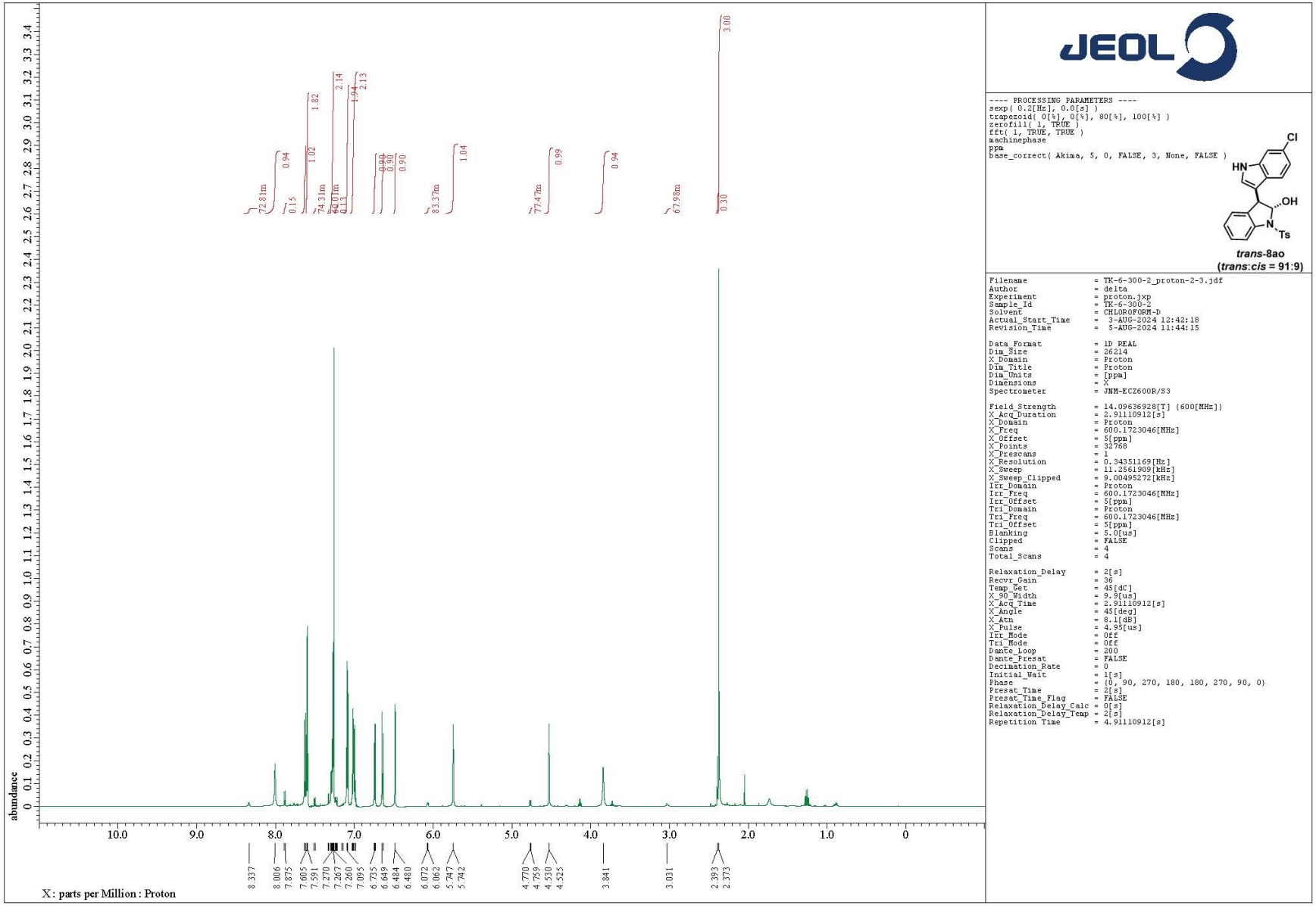



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FALSE )
```


***trans*-8an**
(***trans*:*cis*** = 81:19)

```
Filename                = TK-6-300-4-1_proton-1-4.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-300-4-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  5-AUG-2024 12:17:16
Revision_Time           =  5-AUG-2024 12:24:04

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[MHz])
X_Acq_Duration          = 2.91110912[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 32768
X_Prescans              = 1
X_Resolution            = 0.34351169[Hz]
X_Sweep                 = 11.2561909[kHz]
X_Sweep_Clipped         = 9.00495272[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_Get                = 45[dC]
X_90_Width              = 9.9[us]
X_Acq_Time              = 2.91110912[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                   = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.91110912[s]
```


(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexpT(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
HN
Cl
OH
N
Ts
trans-8an
(trans:cis = 81:19)
Filename = TK-6-122-1-5-2_carbon-2-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-122-1-5-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-JUN-2024 22:37:31
Revision_Time = 27-JUN-2024 23:14:27
Data_Format = 1D COMPLEX
Dim_Size = 2624
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-EC2600R/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 = 128
Total_Scans = 128
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_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = FALSE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Tempi = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]

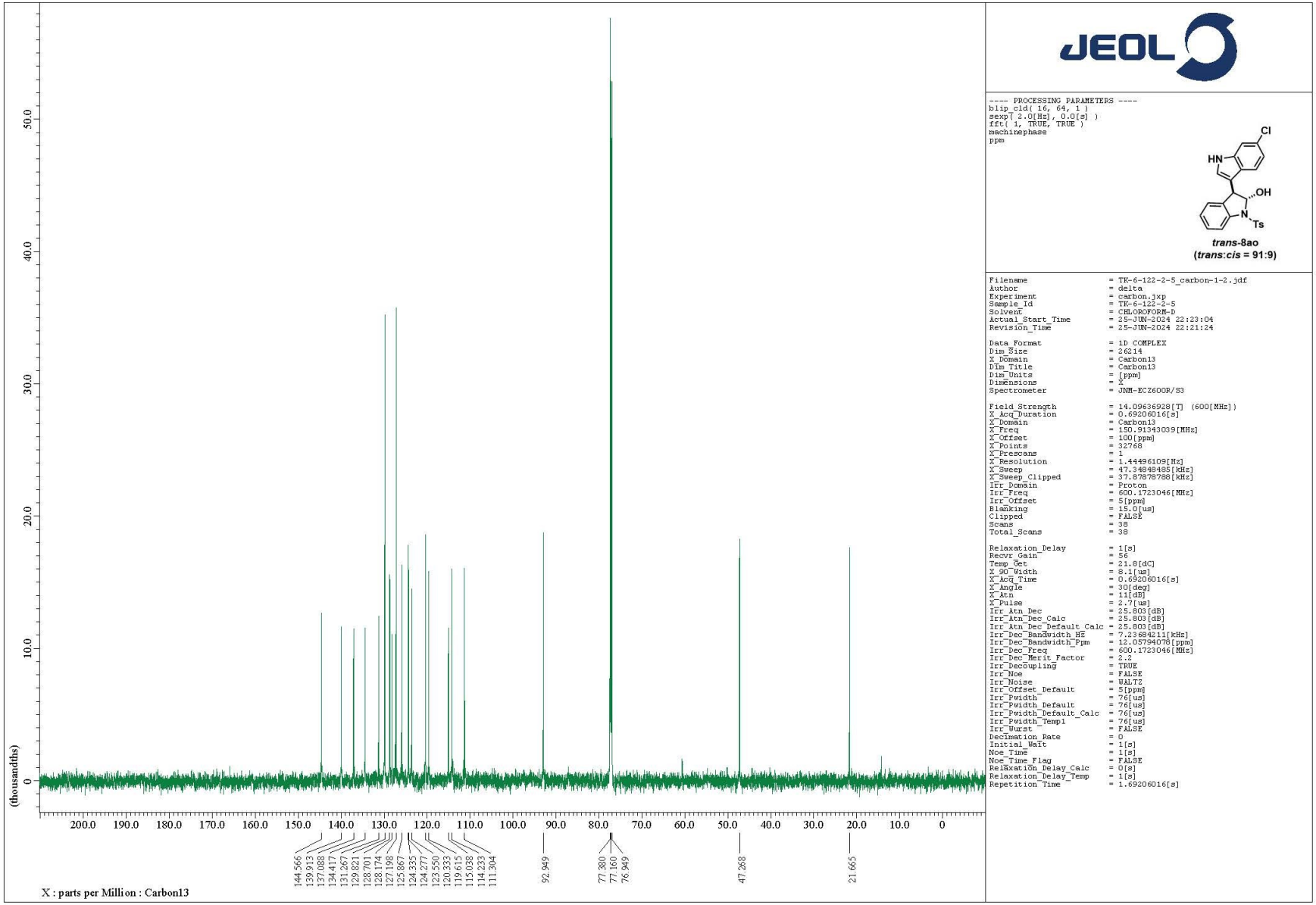


JEOL

```
---- 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, FALSE )
```


***trans*-8ao**
(***trans*:*cis* = 91:9)

```
Filename              = TK-6-300-2_proton-2-3.jdf
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TK-6-300-2
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  3-AUG-2024 12:42:18
Revision_Time         =  5-AUG-2024 11:44:15

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[MHz])
X_Acq_Duration        = 2.91110912[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.34351169[Hz]
X_Sweep               = 11.2561909[kHz]
X_Sweep_Clipped       = 9.00495272[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_Get              = 45[dC]
X_90_Width            = 9.9[us]
X_Acq_Time            = 2.91110912[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                 = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time           = 2[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time       = 4.91110912[s]
```

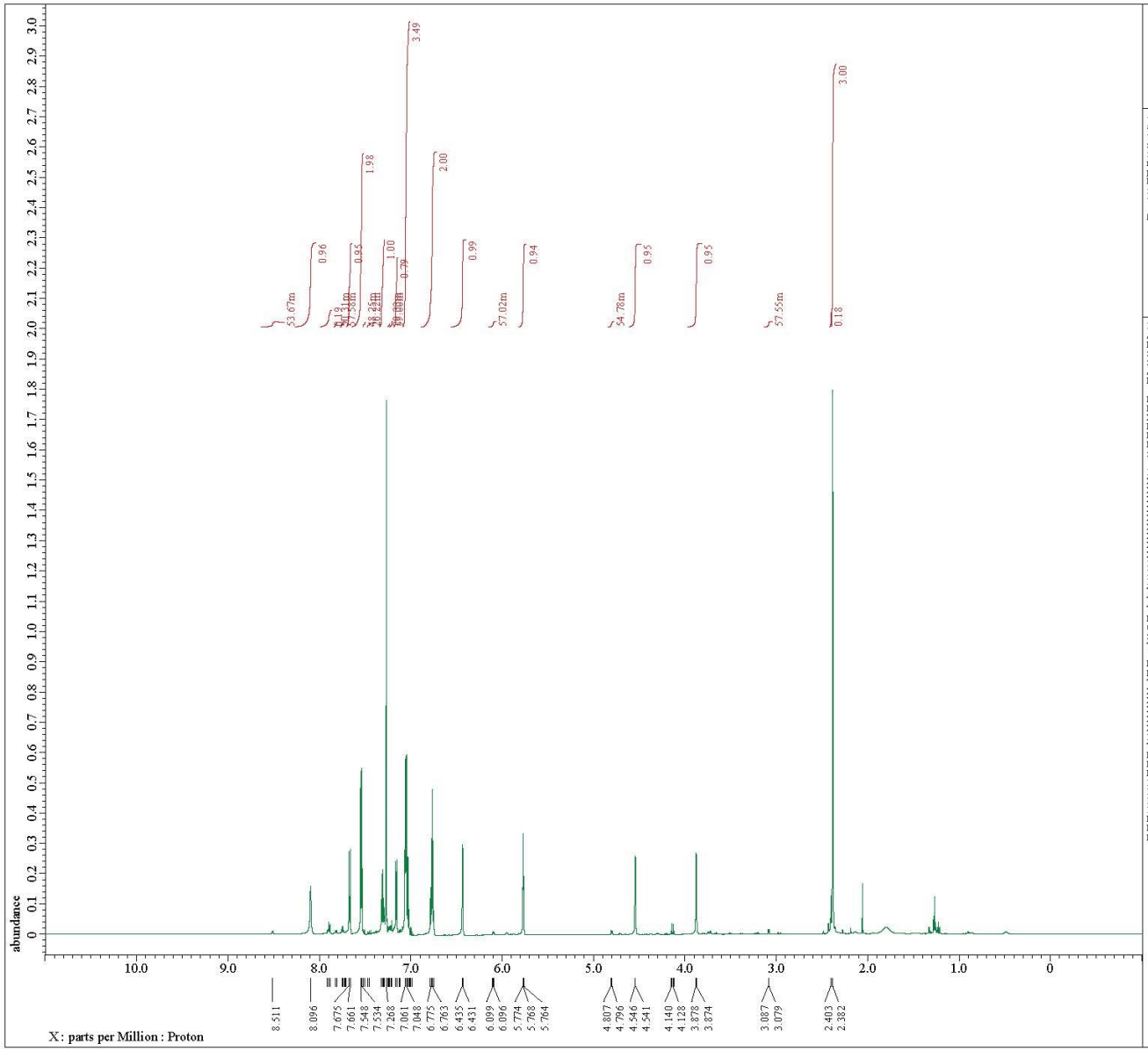


JEOL

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

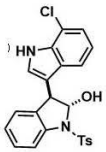

***trans*-8ao**
(***trans*:*cis* = 91:9)

Filename	= TK-6-122-2-5_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-122-2-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2024 22:23:04
Revision_Time	= 25-JUN-2024 22:21:24
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	= 38
Total_Scans	= 38
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21.8[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_Dec_Bandwidth_Hz	= 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



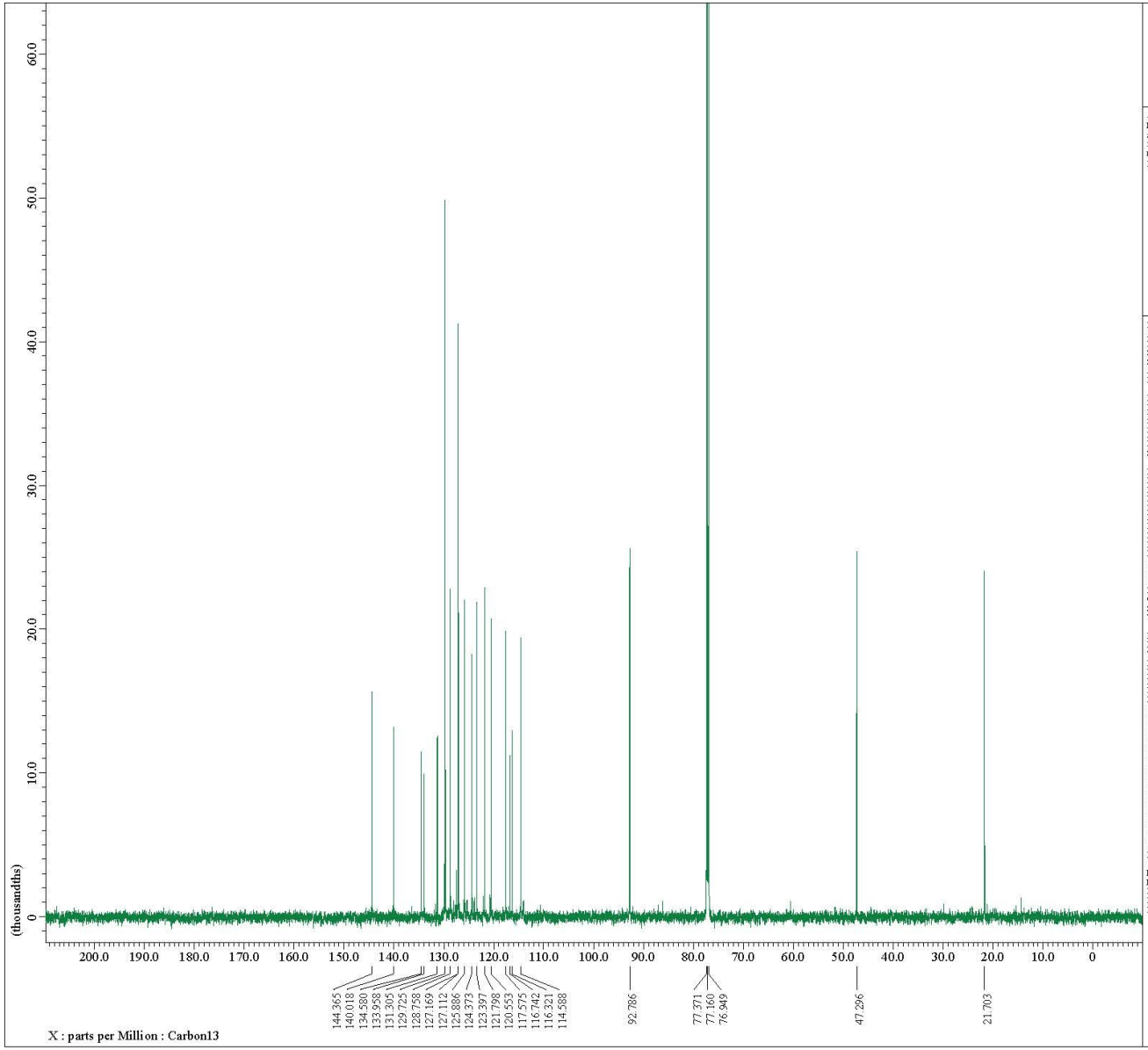
JEOL

```
---- 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, FALSE )
reference( 7.23948[ppm], 7.26[ppm] )
thresh( 0.36547[%], 1, )

以下位由来:: TK-6-122-3-10_proton-2-1.jdf
```

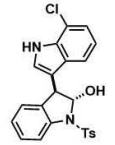


***trans*-8ap**
(*trans*:*cis* = 94:6)

```
Filename                = TK-6-122-3-10_proton-2-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-122-3-10
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  1-JUL-2024 19:44:42
Revision_Time           =  5-AUG-2024 11:52:11

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[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              = 36
Temp_Get                = 21[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                   = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```

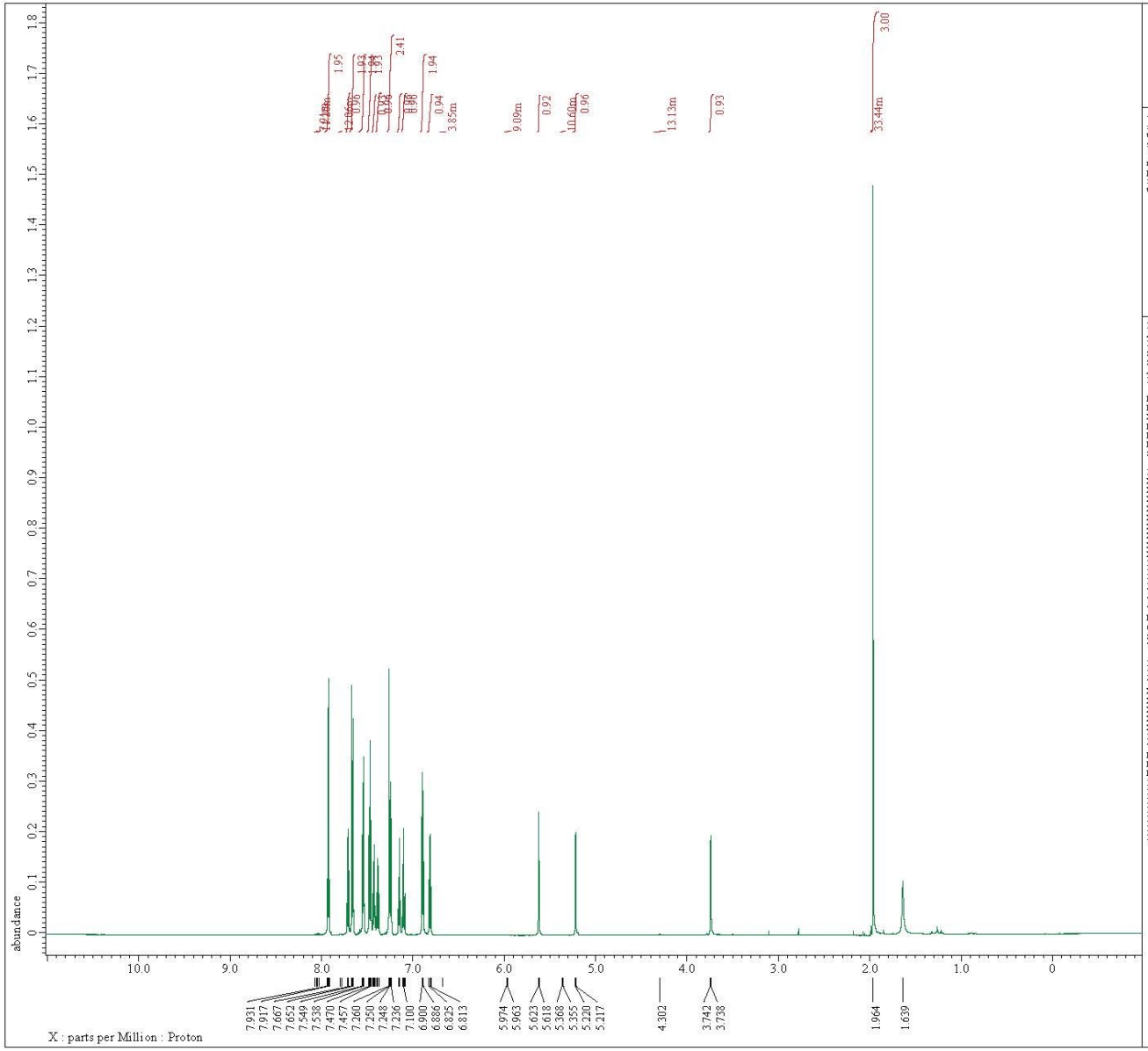


---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm



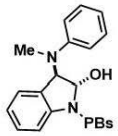
***trans*-8ap**
(***trans*:*cis*** = 94:6)

Filename	= TK-6-122-3-10_carbon-2-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-122-3-10
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-JUL-2024 19:45:29
Revision_Time	= 1-JUL-2024 19:44:55
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-EC2600R/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	= 64
Total_Scans	= 64
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



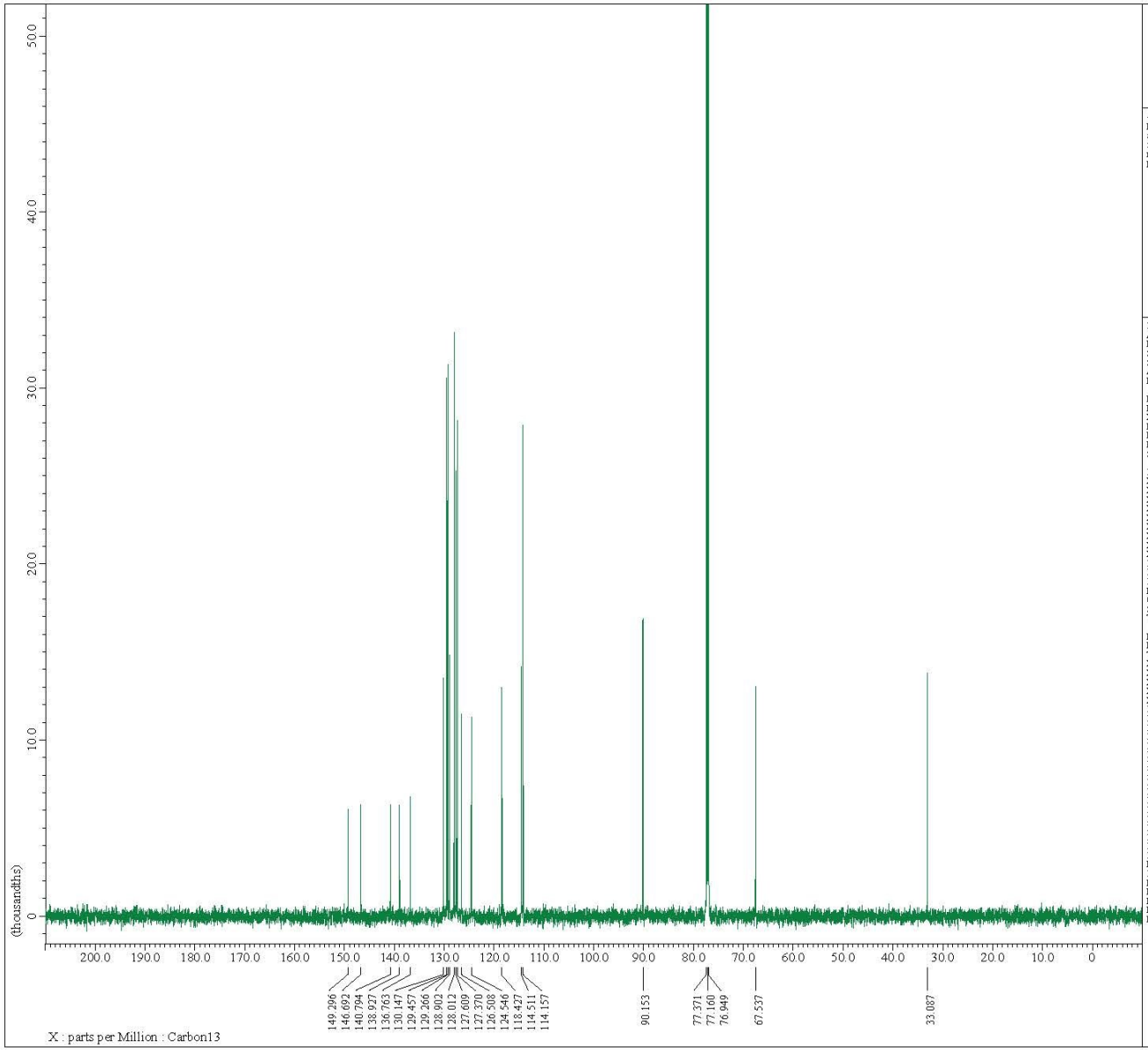
JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.24864[ppm], 7.26[ppm] )
thresh( 3.26468[%], 1, )
```



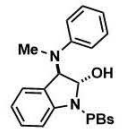
***trans*-8la**
(***trans*:*cis*** = 99:1)

```
Filename                = KY-1-069-6_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = KY-1-069-6
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 20-JUN-2024 22:48:42
Revision_Time           =  5-AUG-2024 12:35:00

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              = 36
Temp_Get                = 21[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                   = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```



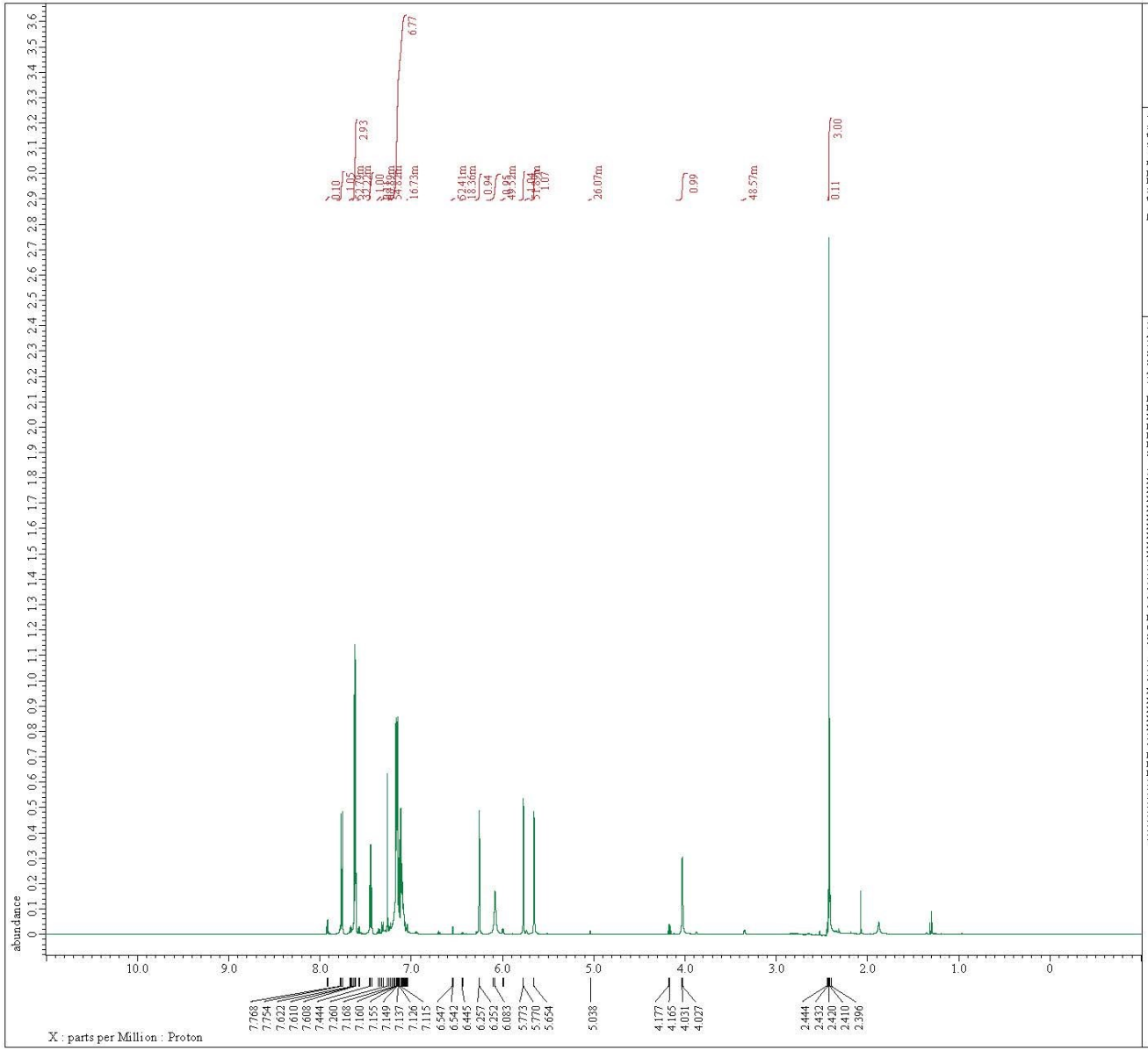
JEOL

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



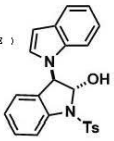
***trans*-8la**
(***trans*:*cis*** = 99:1)

Filename	= KY-1-069-6_carbon-1-3.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-1-069-6
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JUN-2024 22:50:44
Revision_Time	= 21-JUN-2024 07:55:18
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	= 57
Total_Scans	= 57
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21[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	= 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Declination_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



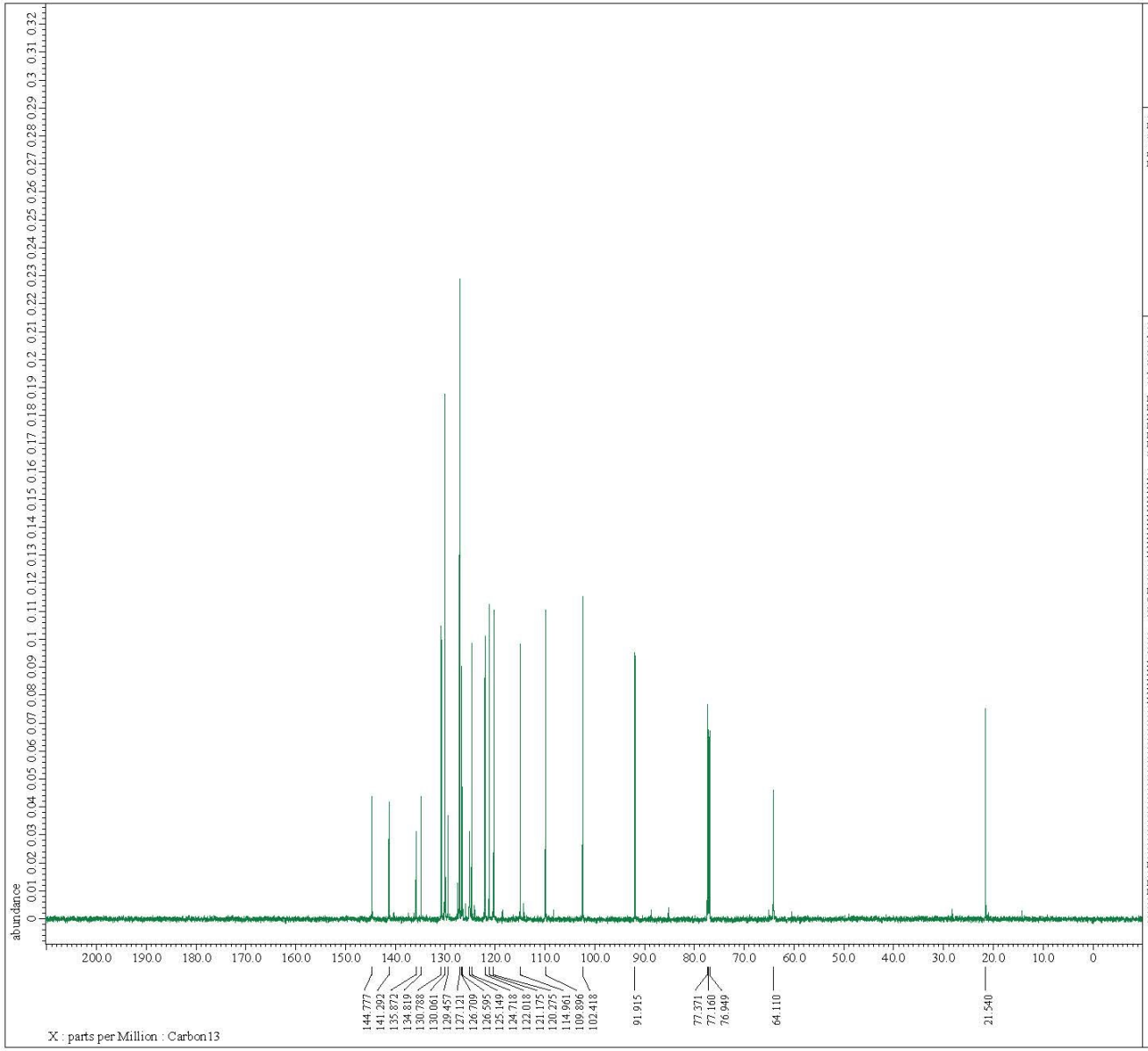
JEOL

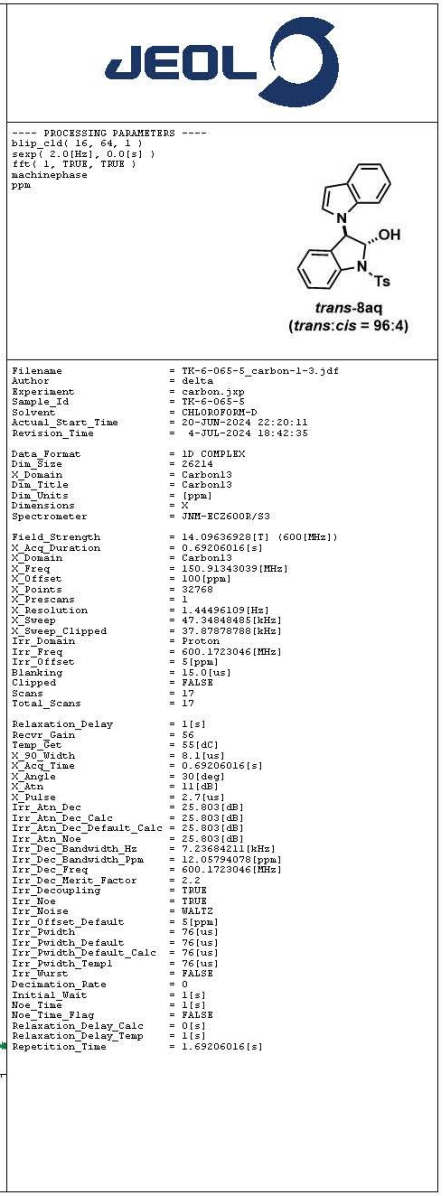
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FALSE )
reference( 7.24558[ppm], 7.26[ppm] )
thresh( 0.62565[%], 1, )

以下由来:: TK-6-065-5 proton-1-1.jdf
```

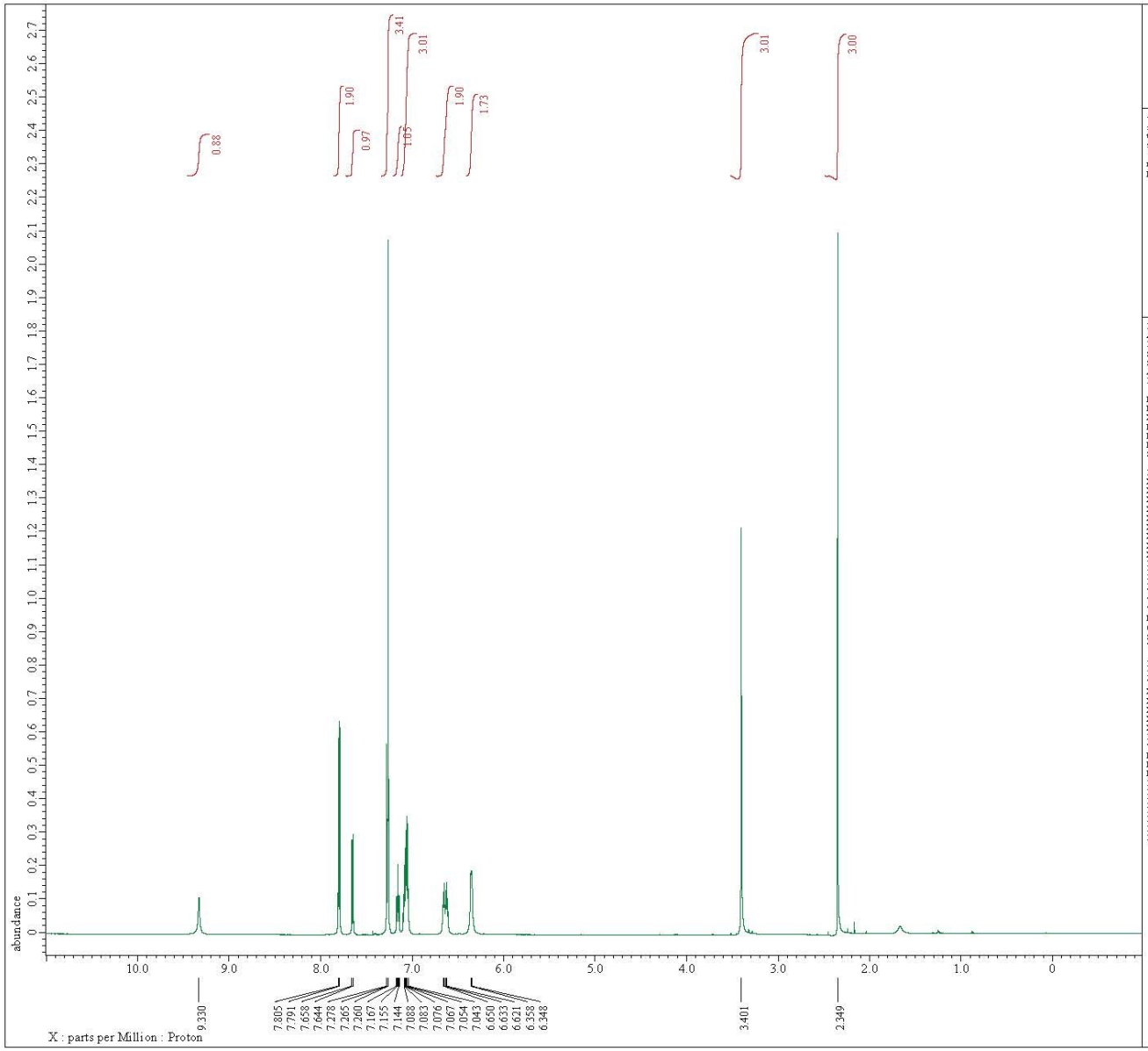


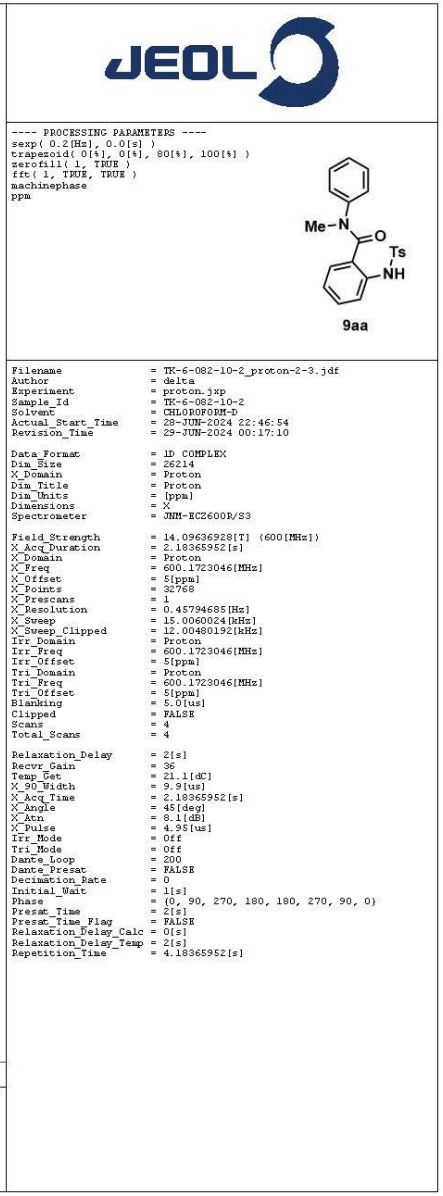
***trans*-8aq**
(***trans*:*cis* = 96:4)

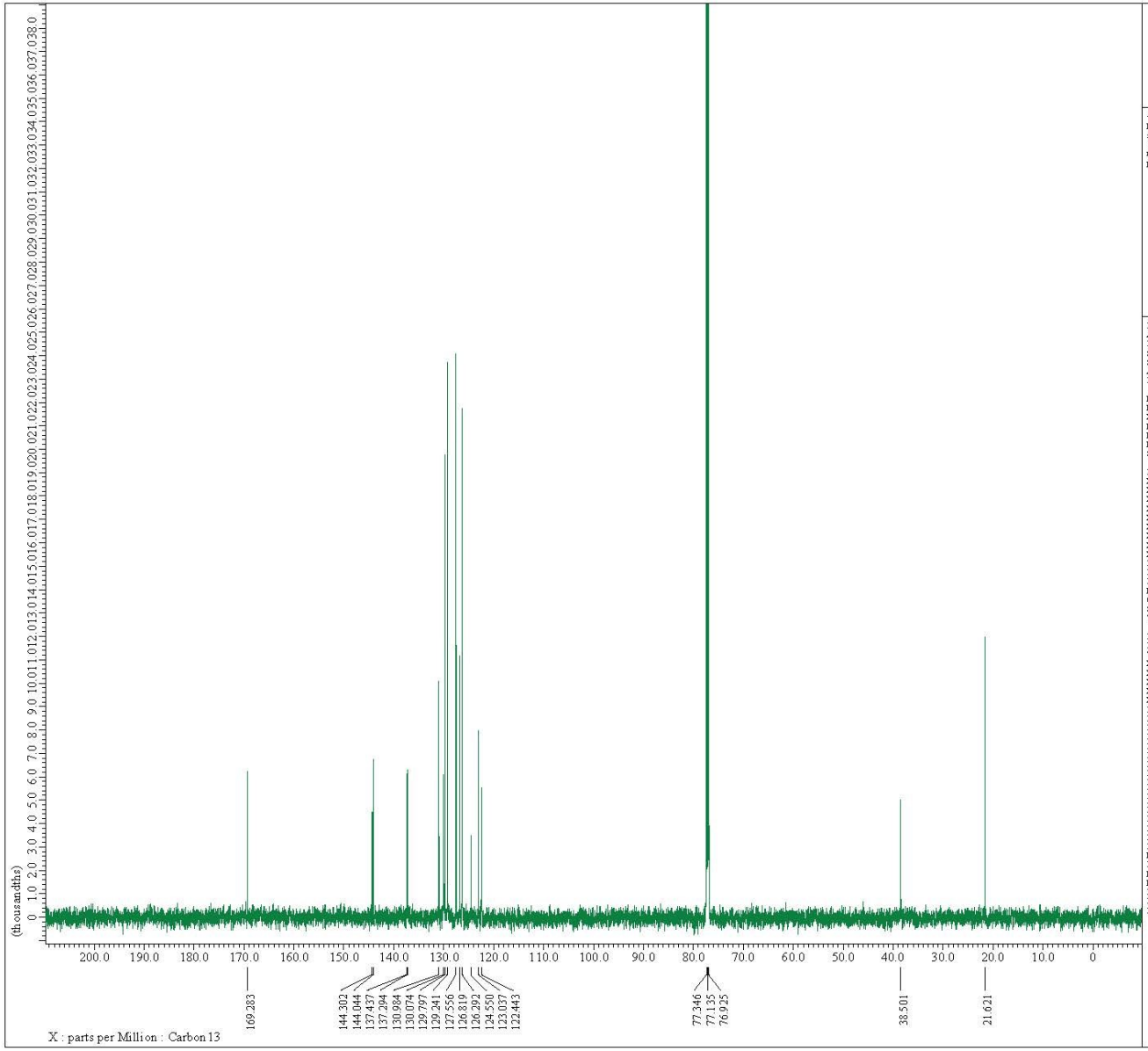
```
Filename                = TK-6-065-5_proton-1-2.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-065-5
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 20-JUN-2024 22:18:04
Revision_Time           =  5-AUG-2024 12:42:49

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[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_Get                = 55[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```


abundance
X : parts per Million : Carbon13
144.777
141.292
135.672
134.819
130.788
130.061
129.457
127.121
126.709
126.595
125.149
124.718
122.018
121.175
120.275
114.961
109.896
102.418
91.915
77.371
77.160
76.949
64.110
21.540

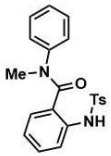

JEOL
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
N
OH
N
Ts
trans-8aq
(trans:cis = 96:4)
Filename = TK-6-065-5_carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-065-5
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-JUN-2024 22:20:11
Revision_Time = 4-JUL-2024 18:42:35
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 = 17
Total_Scans = 17
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 55[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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]


abundance
X : parts per Million : Proton
0.88
1.90
0.97
3.41
3.01
1.05
1.90
1.73
3.01
3.00
9.330
7.805
7.791
7.658
7.644
7.278
7.265
7.260
7.167
7.155
7.144
7.088
7.083
7.076
7.067
7.054
7.043
6.650
6.633
6.621
6.358
6.348
3.401
2.349


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Me-N
O
Ts
NH
9aa
Filename = TK-6-082-10-2_proton-2-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-082-10-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-JUN-2024 22:46:54
Revision_Time = 29-JUN-2024 00:17:10
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 = 36
Temp_Get = 21.1[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 = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18365952[s]

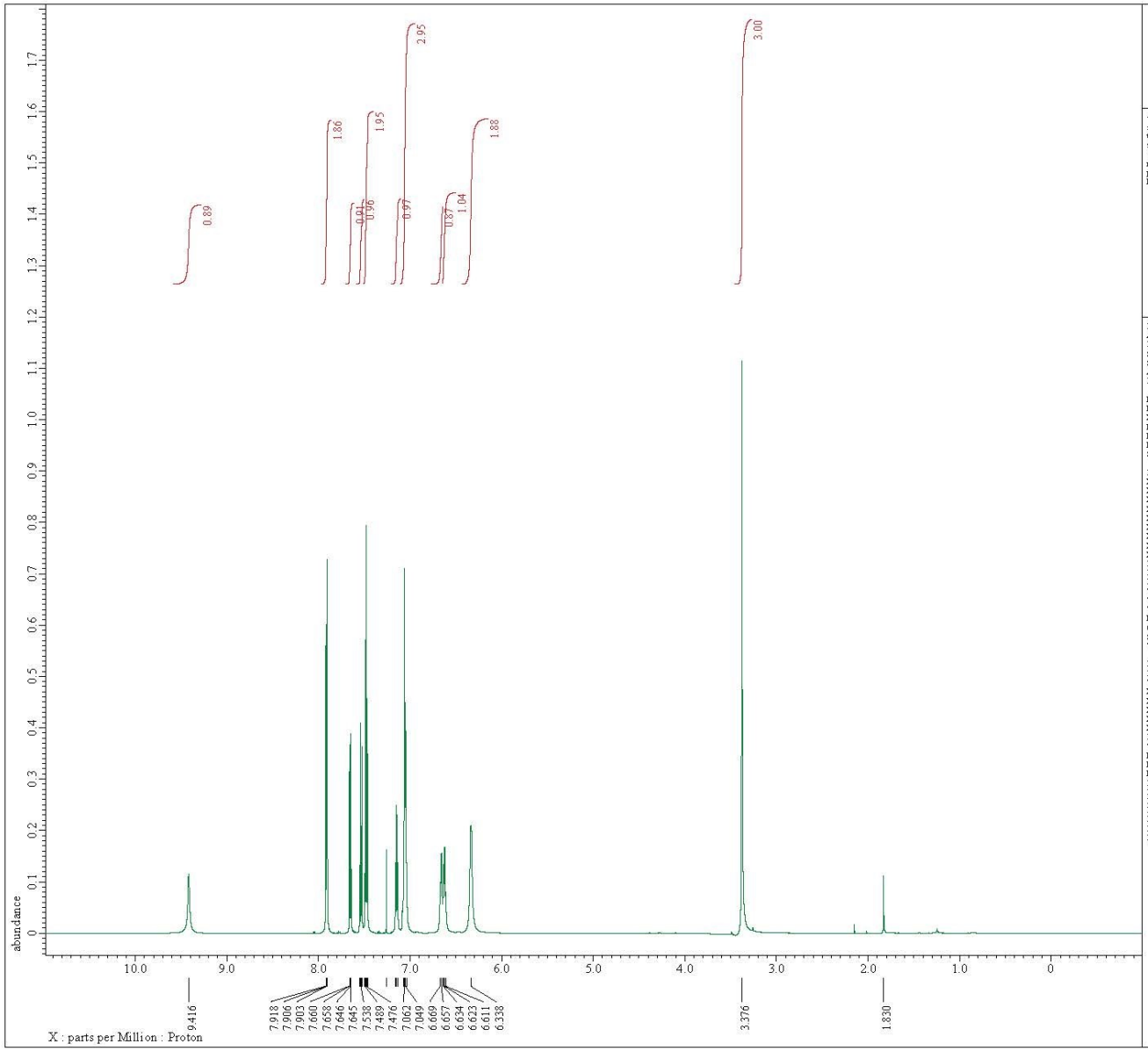


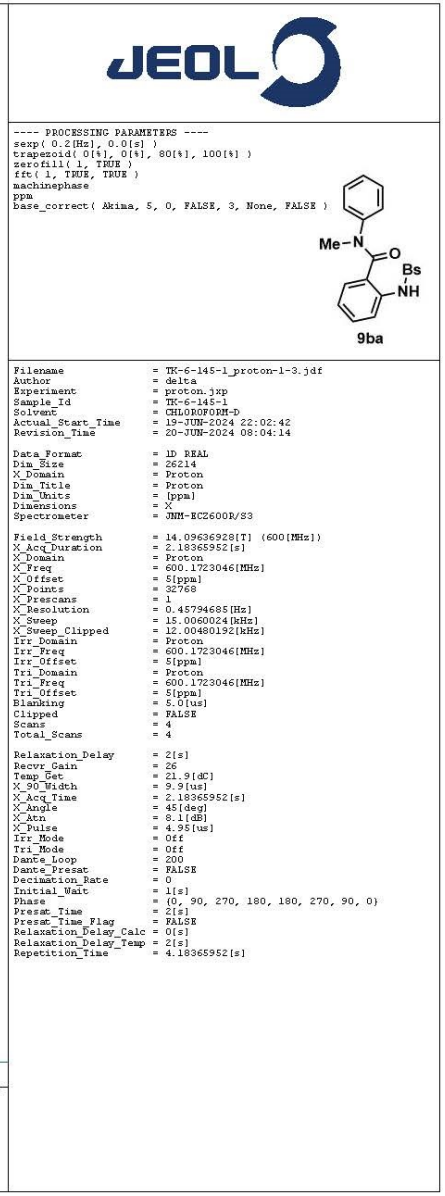
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm

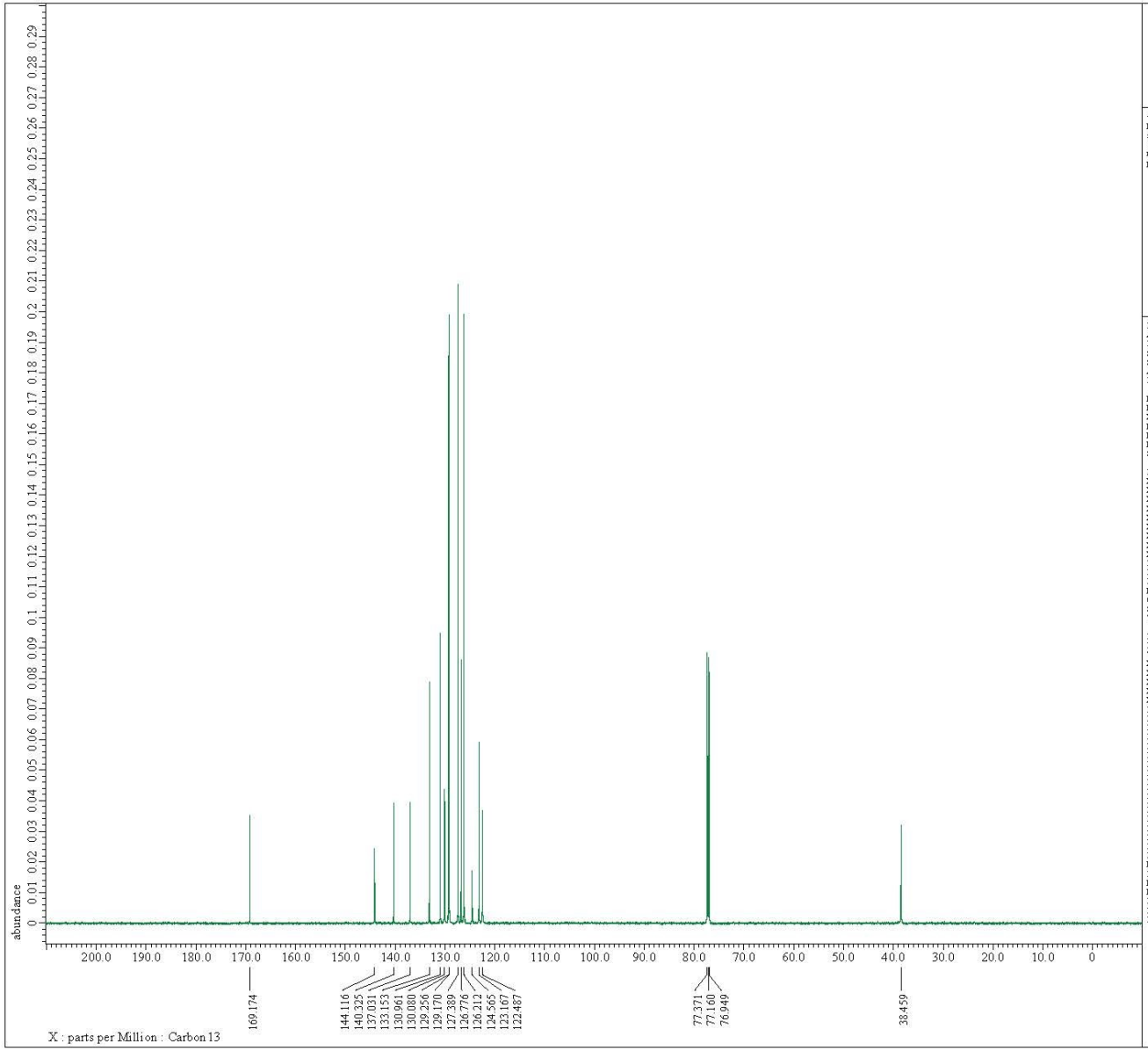


9aa

Filename	= TK-6-082-10-2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-082-10-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-JUN-2024 22:47:40
Revision_Time	= 28-JUN-2024 23:00:21
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	= 64
Total_Scans	= 64
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 21[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_Dec_Bandwidth_Hz	= 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

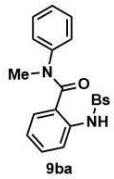

abundance
X : parts per Million : Proton
9.416
7.918
7.906
7.903
7.660
7.658
7.646
7.645
7.538
7.489
7.476
7.062
7.049
6.669
6.657
6.634
6.623
6.611
6.338
3.376
1.830
0.89
1.86
0.91
0.96
1.95
0.97
2.95
0.87
1.04
1.88
3.00


JEOL
---- 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, FALSE)
Me-N
O
Bs
NH
9ba
Filename = TK-6-145-1_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-145-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2024 22:02:42
Revision_Time = 20-JUN-2024 08:04:14
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[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_Get = 21.9[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 = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18365952[s]



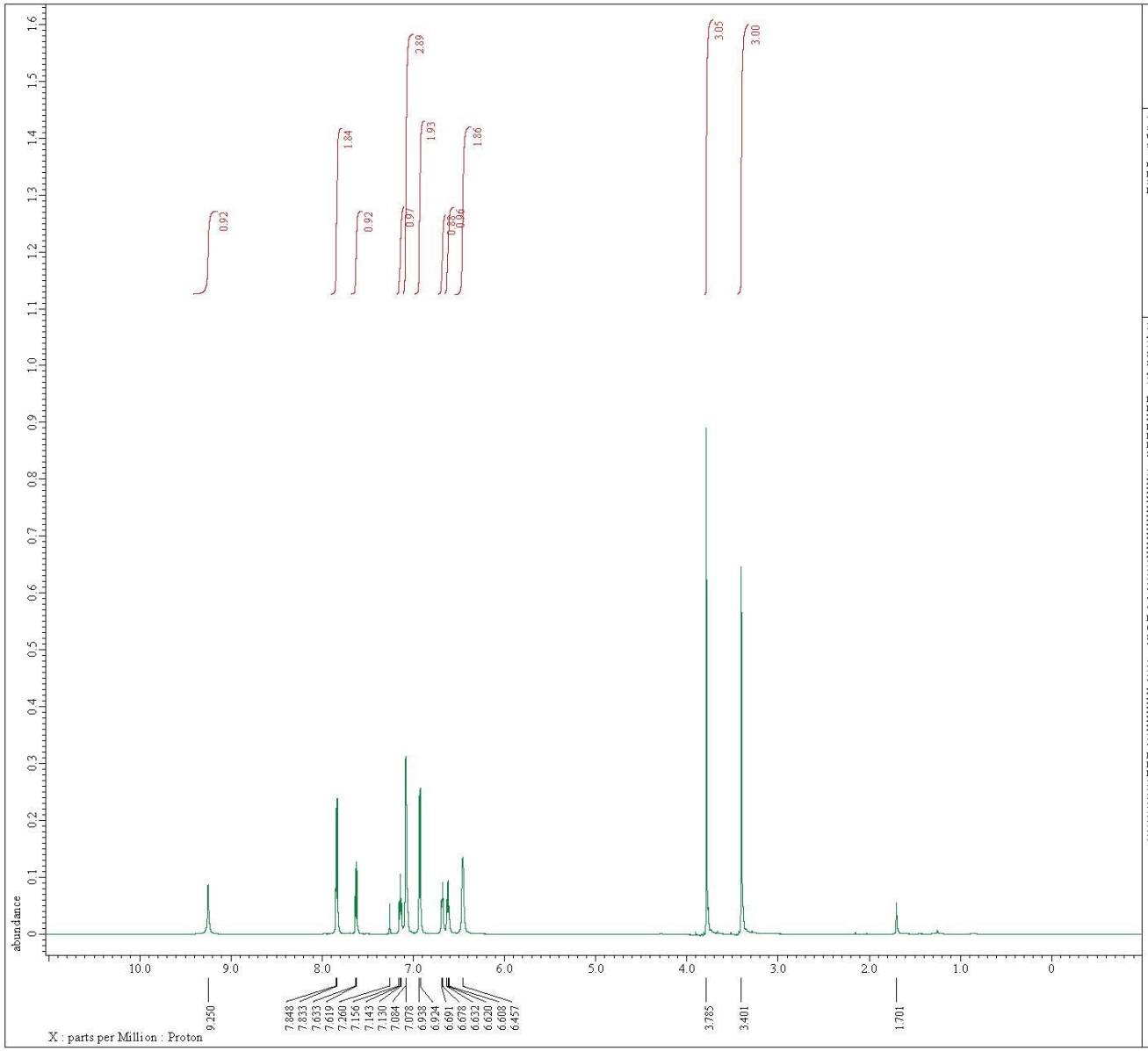
JEOL

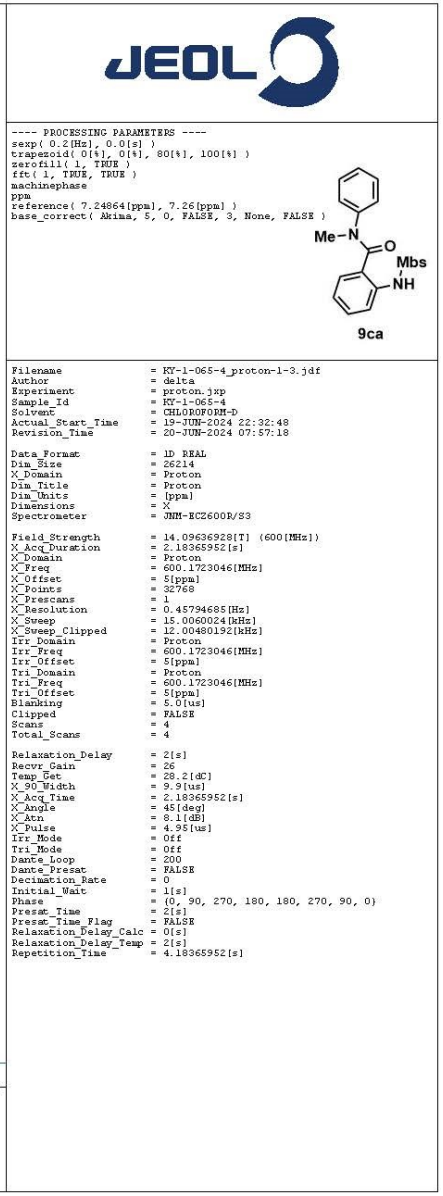
```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

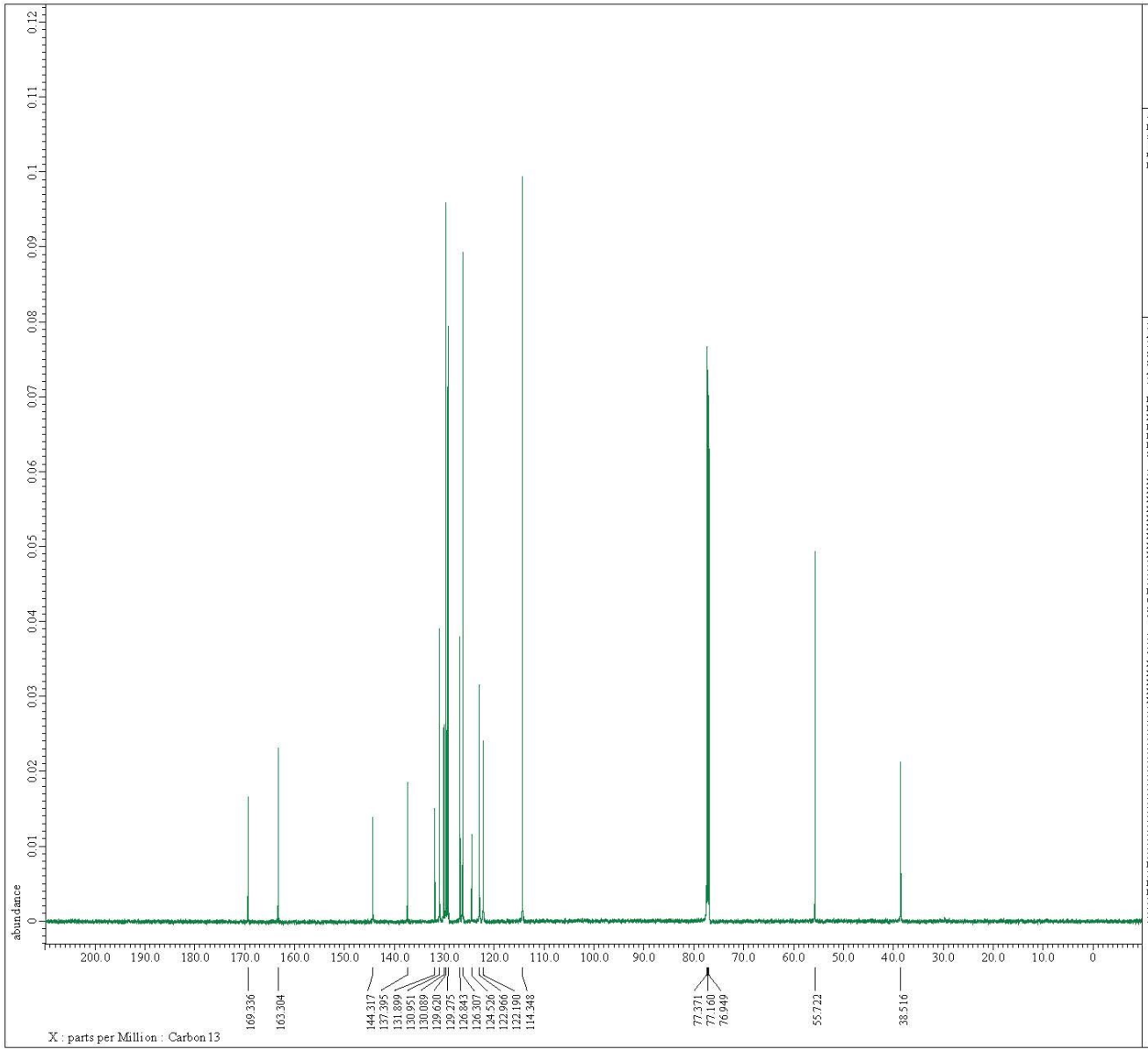


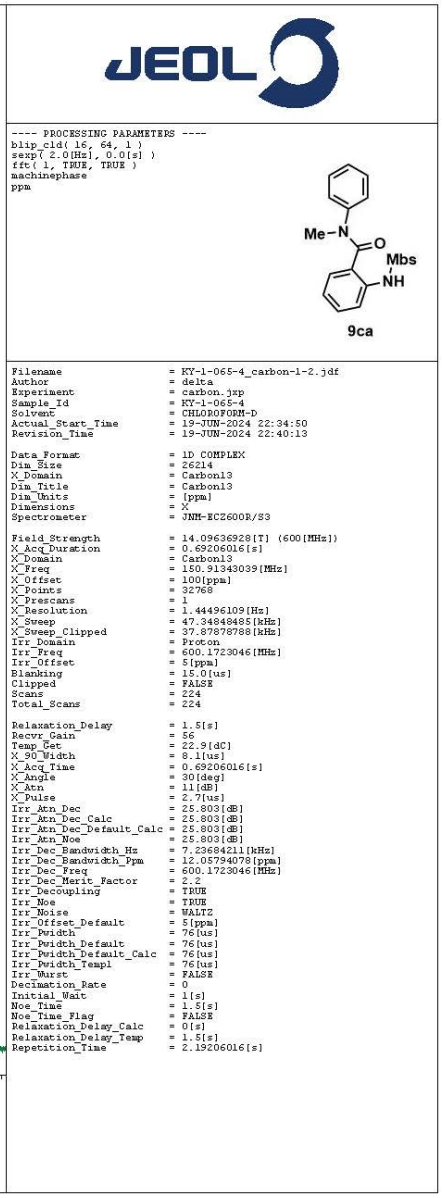
9ba

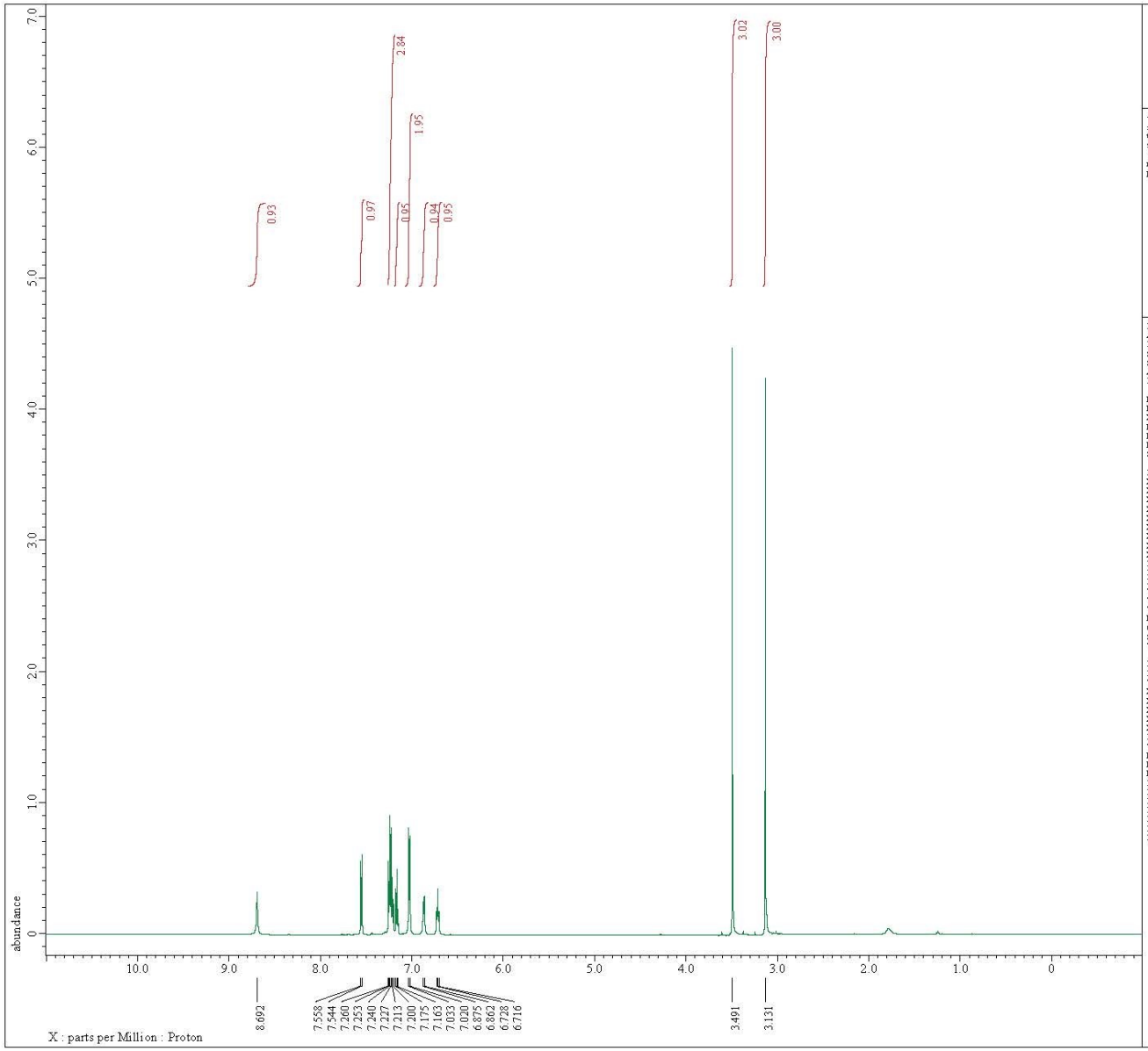
Filename	= TK-6-145-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-145-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-JUN-2024 22:04:44
Revision_Time	= 19-JUN-2024 22:13:01
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 165
Total_Scans	= 165
Relaxation_Delay	= 1.5[s]
Recvr_Gain	= 56
Temp_Get	= 20.7[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	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1.5[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1.5[s]
Repetition_Time	= 2.19206016[s]


abundance
X : parts per Million : Proton
0.92
1.84
0.92
2.89
0.97
1.93
0.88
0.96
1.86
3.05
3.00
9.250
7.848
7.833
7.633
7.619
7.260
7.156
7.143
7.130
7.084
7.078
6.938
6.924
6.691
6.678
6.632
6.620
6.608
6.457
3.785
3.401
1.701


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(7.24864[ppm], 7.26[ppm])
base_correct(Akima, 5, 0, FALSE, 3, None, FALSE)
Me-N
O
Mbs
NH
9ca
Filename = KY-1-065-4_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = KY-1-065-4
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2024 22:32:48
Revision_Time = 20-JUN-2024 07:57:18
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[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_Get = 28.2[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 = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
RelaxationDelay_Calc = 0[s]
RelaxationDelay_Temp = 2[s]
Repetition_Time = 4.18365952[s]

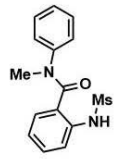

abundance
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
169.336
163.304
144.317
137.395
131.899
130.951
130.089
129.620
129.275
126.843
126.307
124.526
122.966
122.190
114.348
77.371
77.160
76.949
55.722
38.516
X : parts per Million : Carbon13


JEOL
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
ffc(1, TRUE, TRUE)
machinephase
ppm
Me-N
O
Mbs
NH
9ca
Filename = KY-1-065-4_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = KY-1-065-4
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2024 22:34:50
Revision_Time = 19-JUN-2024 22:40:13
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 = 150.91343039[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 = 224
Total_Scans = 224
Relaxation_Delay = 1.5[s]
Recvr_Gain = 56
Temp_Get = 22.9[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 = 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1.5[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1.5[s]
Repetition_Time = 2.19206016[s]



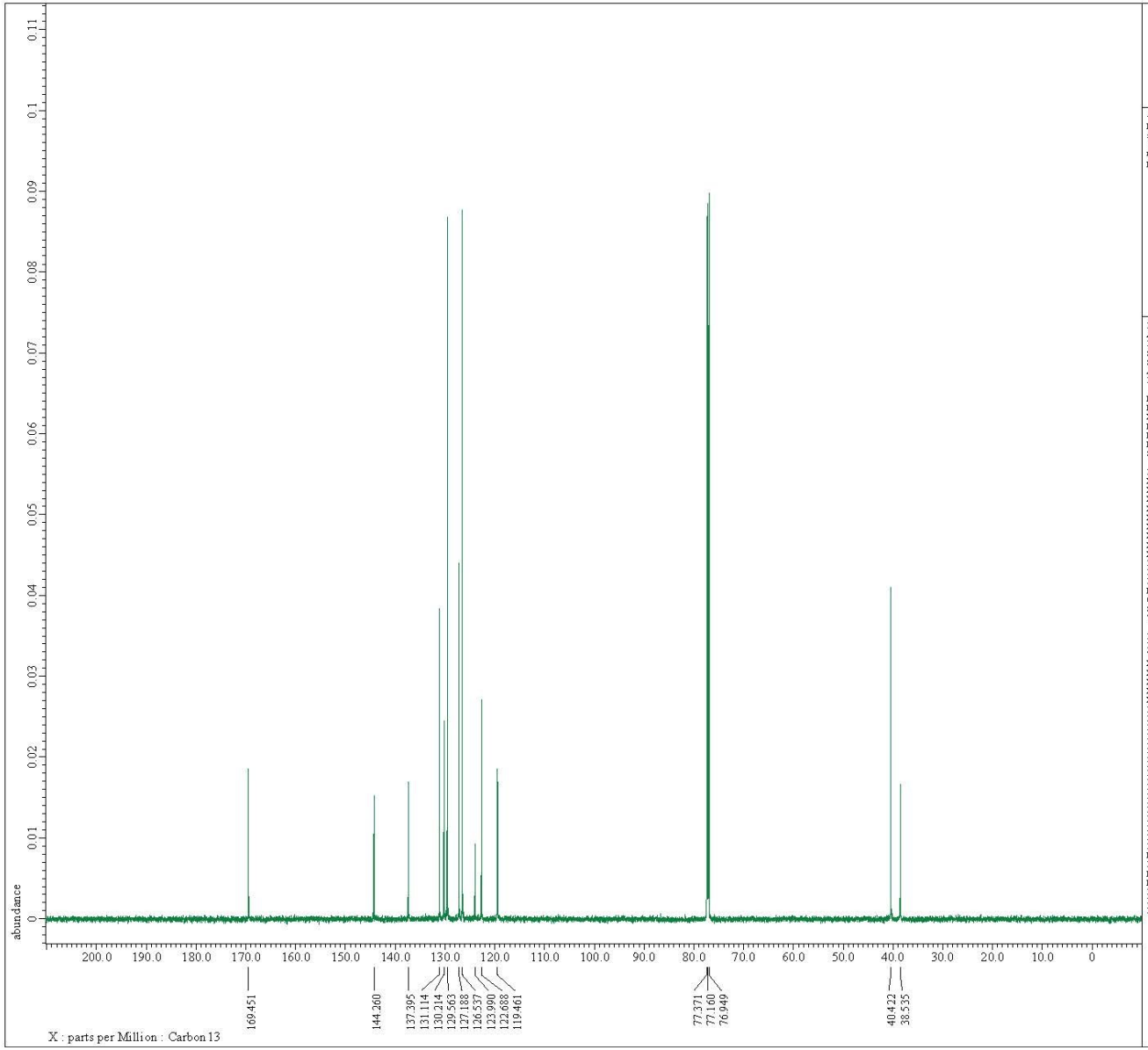
JEOL

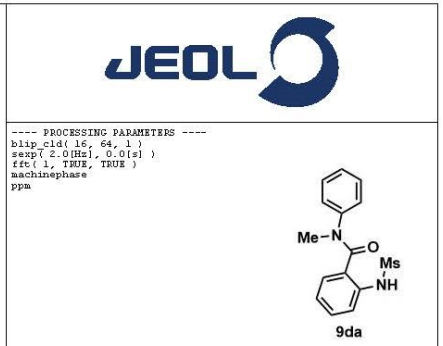
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```



9da

Filename	= TK-6-150-1_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-6-150-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-JUN-2024 21:10:58
Revision_Time	= 24-JUN-2024 23:02:56
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	= 36
Temp_Get	= 21[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	= (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.18365952[s]

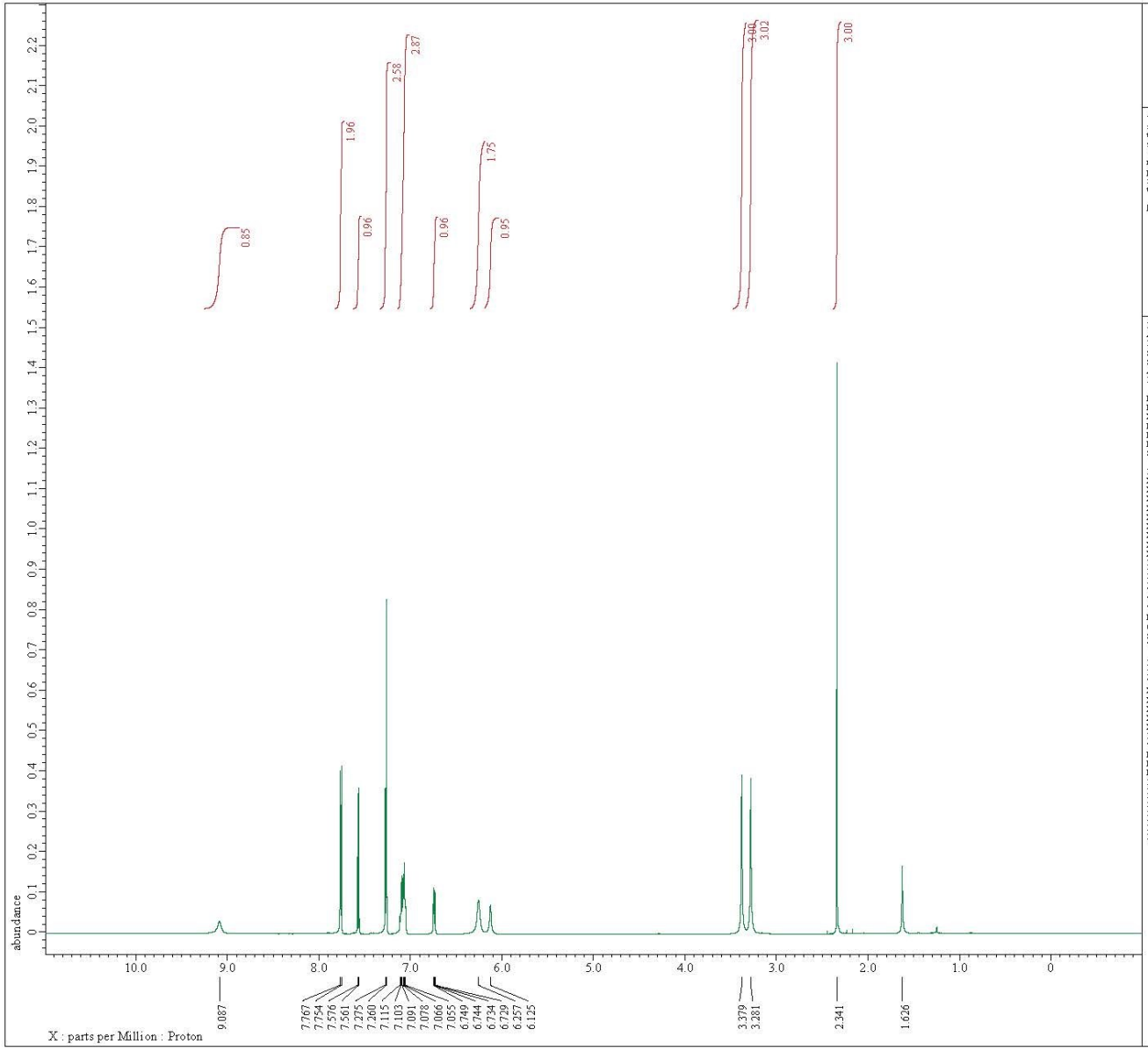




9da

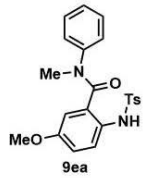
```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= TK-6-150-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-150-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-JUN-2024 21:11:45
Revision_Time	= 24-JUN-2024 21:12:13
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	= 150.91343039[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	= 21[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



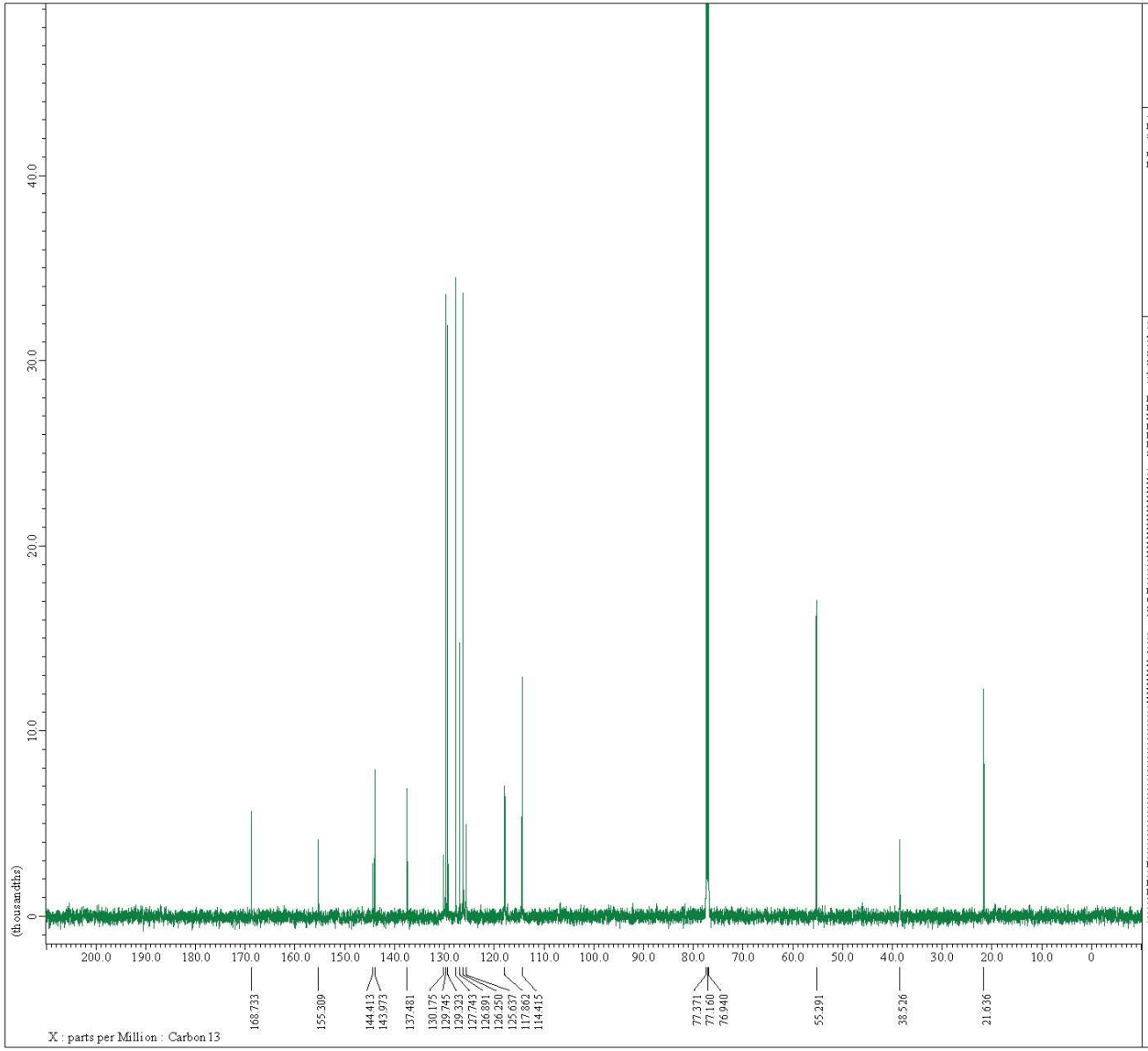
JEOL

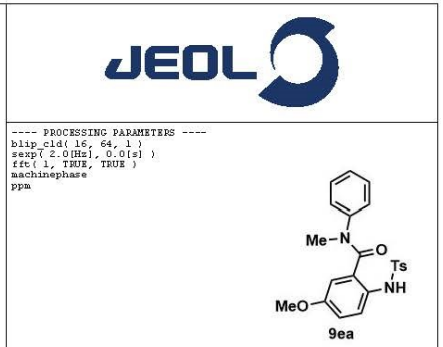
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.24864[ppm], 7.26[ppm] )
thresh( 1.32653[%], 1, )

以下由来:: KY-1-050-2 proton-1-1.jdf
```



9ea

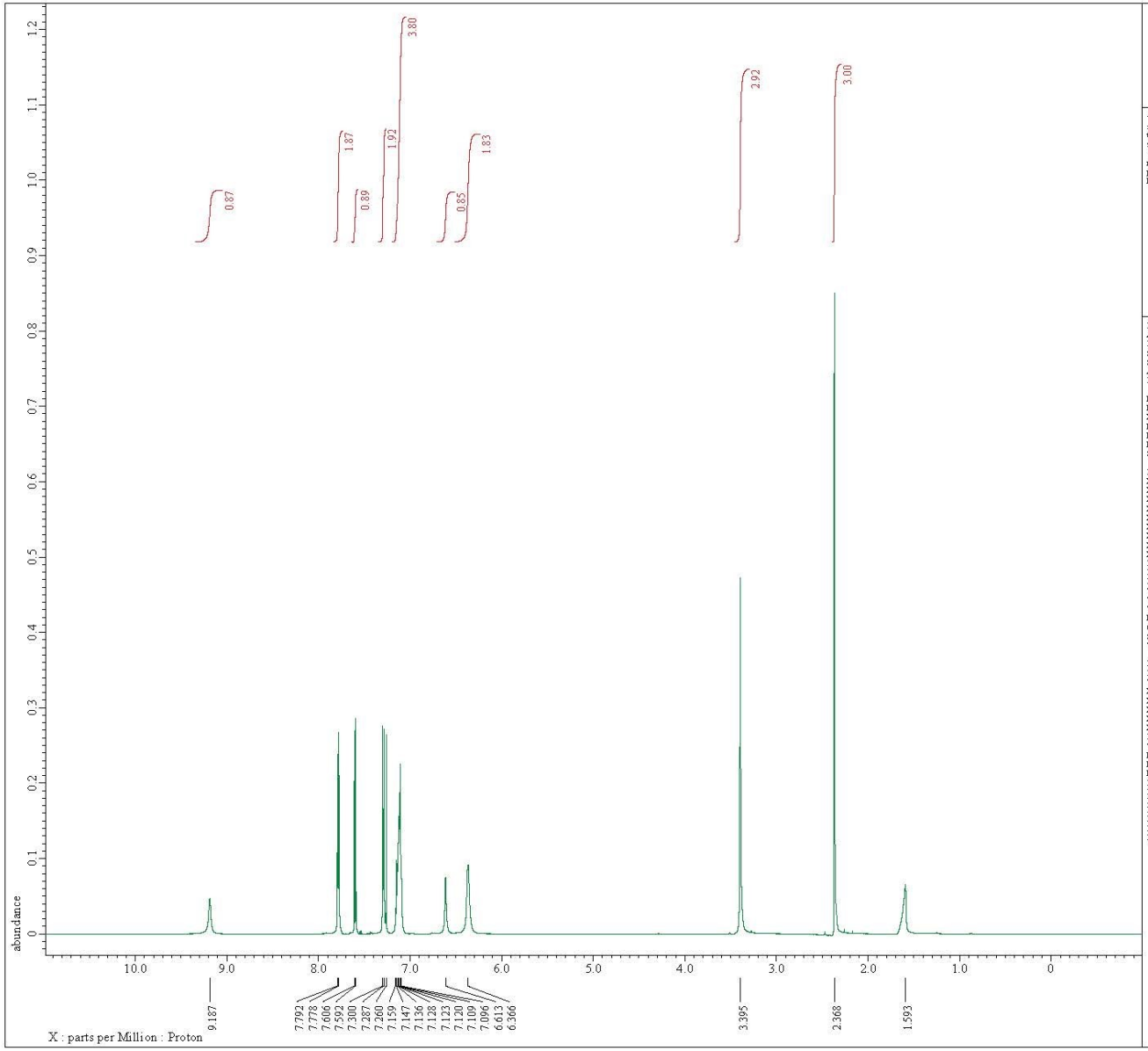
Filename	= KY-1-050-2_proton-1-2.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= KY-1-050-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JUN-2024 22:34:03
Revision_Time	= 21-JUN-2024 08:06:00
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= 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	= 36
Temp_Set	= 21.5[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	= {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.18365952[s]





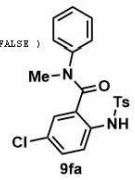

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= KY-1-050-2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-1-050-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JUN-2024 22:36:06
Revision_Time	= 20-JUN-2024 22:35:52
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	= 71
Total_Scans	= 71
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 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	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



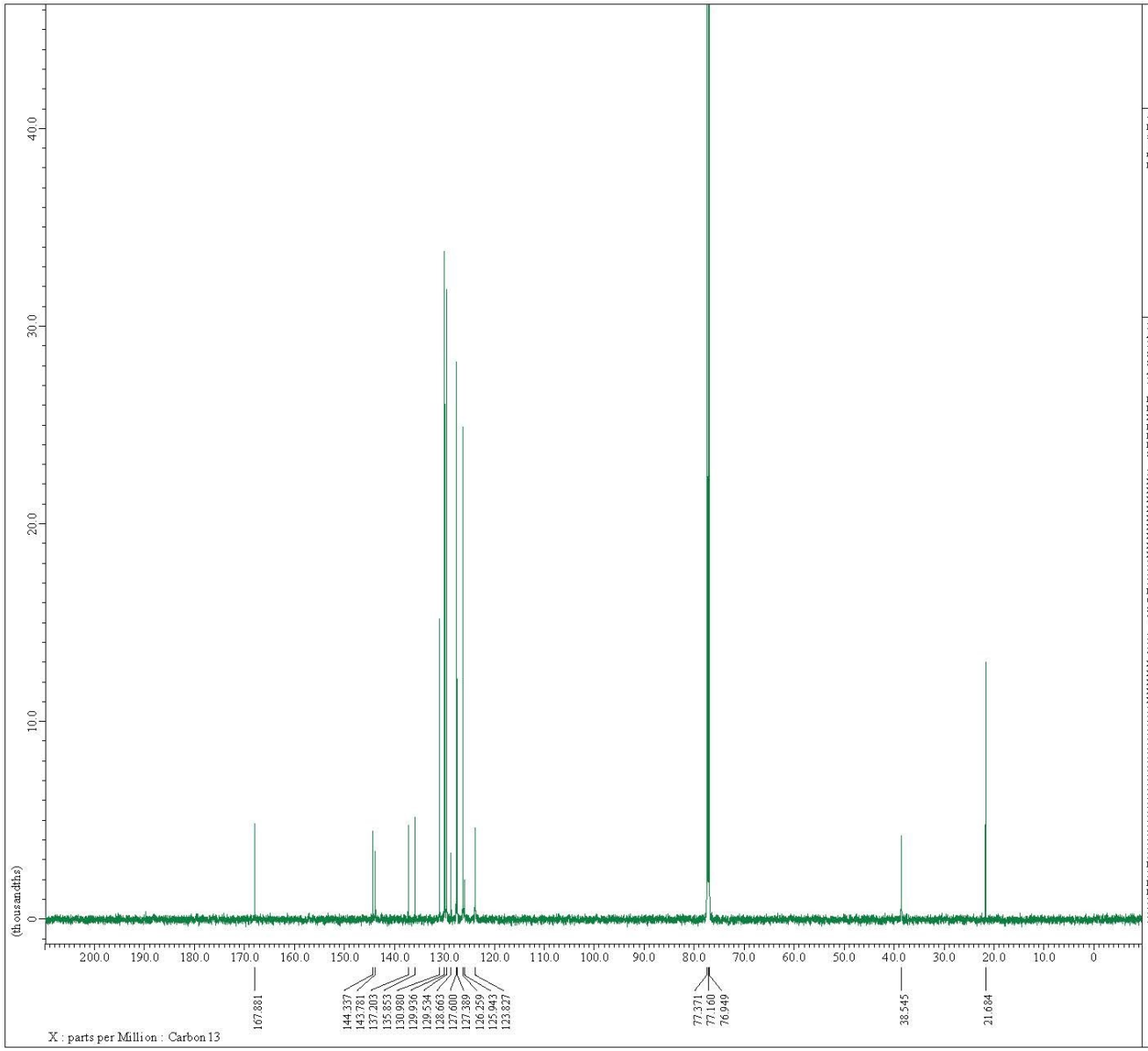
JEOL

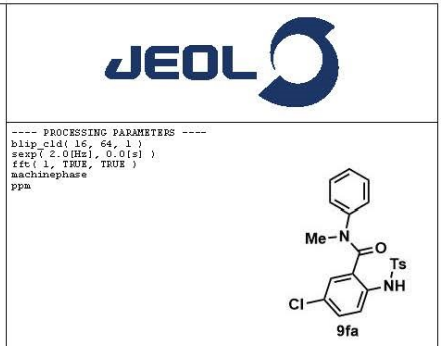
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FALSE )
```



9fa

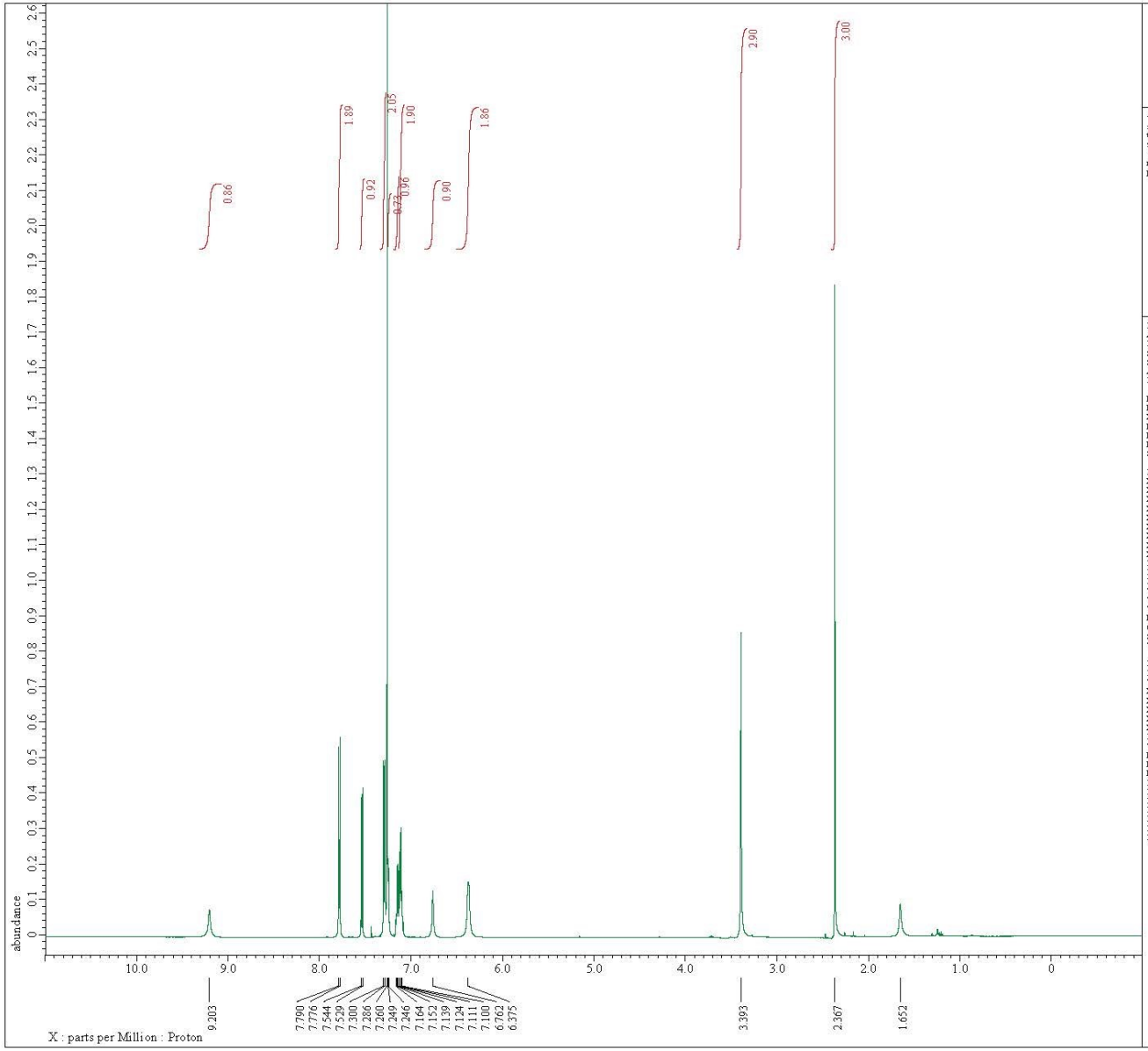
```
Filename                = KY-1-053-5_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = KY-1-053-5
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 23-JUN-2024 13:25:00
Revision_Time           = 24-JUN-2024 08:06:03

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[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              = 36
Temp_Set                = 21.9[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```

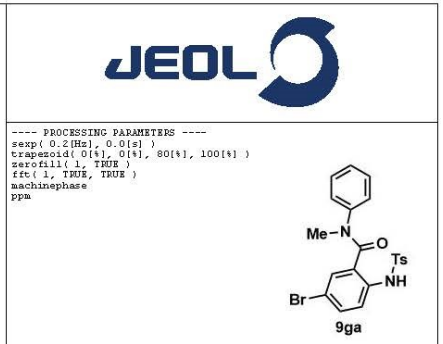





```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

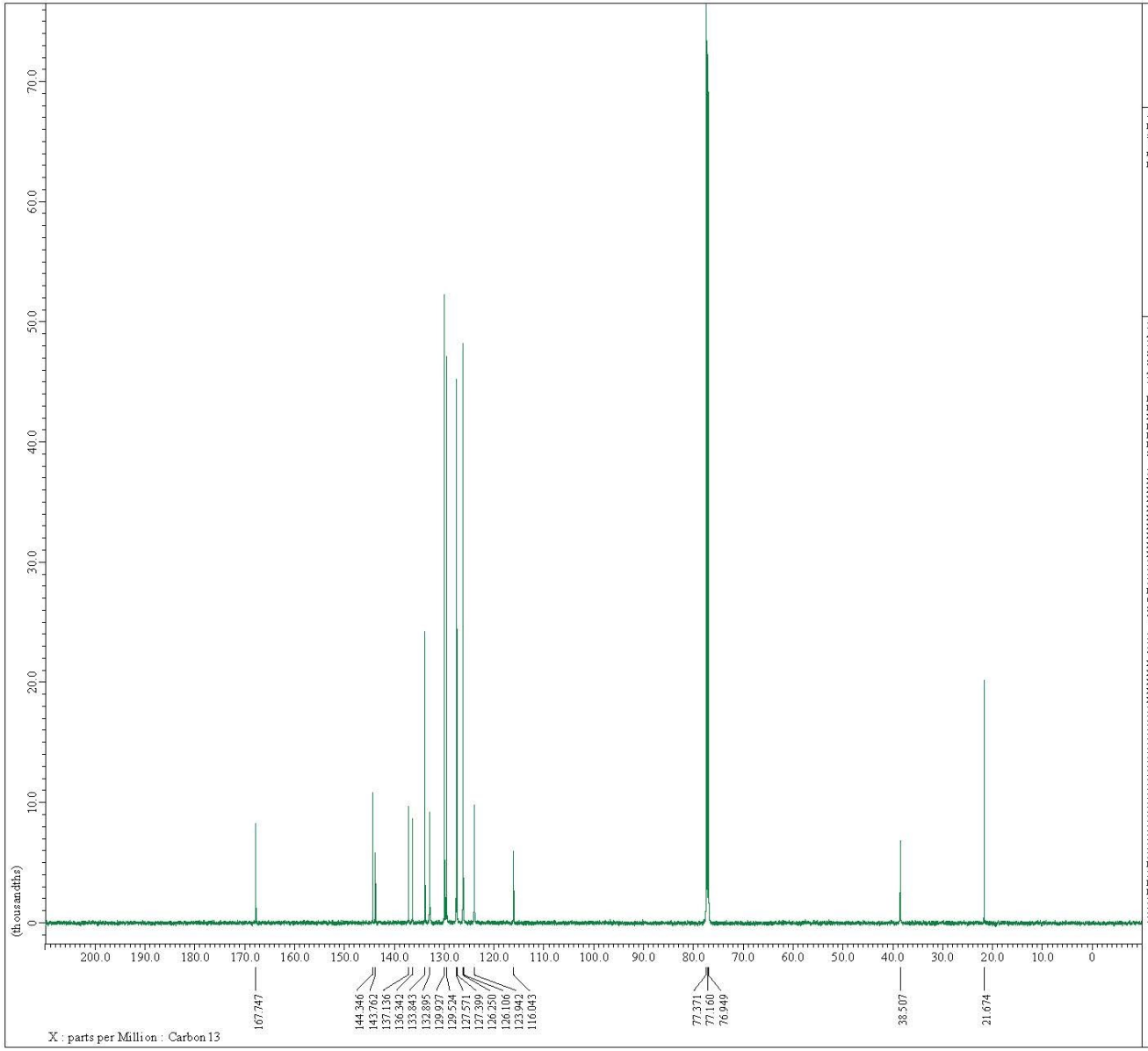
Filename	= KY-1-053-5_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-1-053-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JUN-2024 13:27:02
Revision_Time	= 23-JUN-2024 13:34:26
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 256
Total_Scans	= 256
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 21[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	= 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

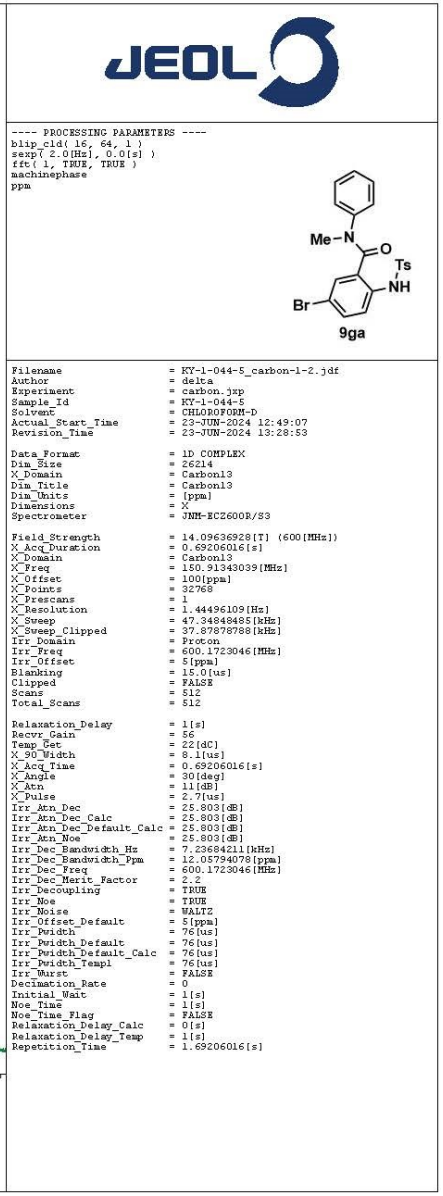


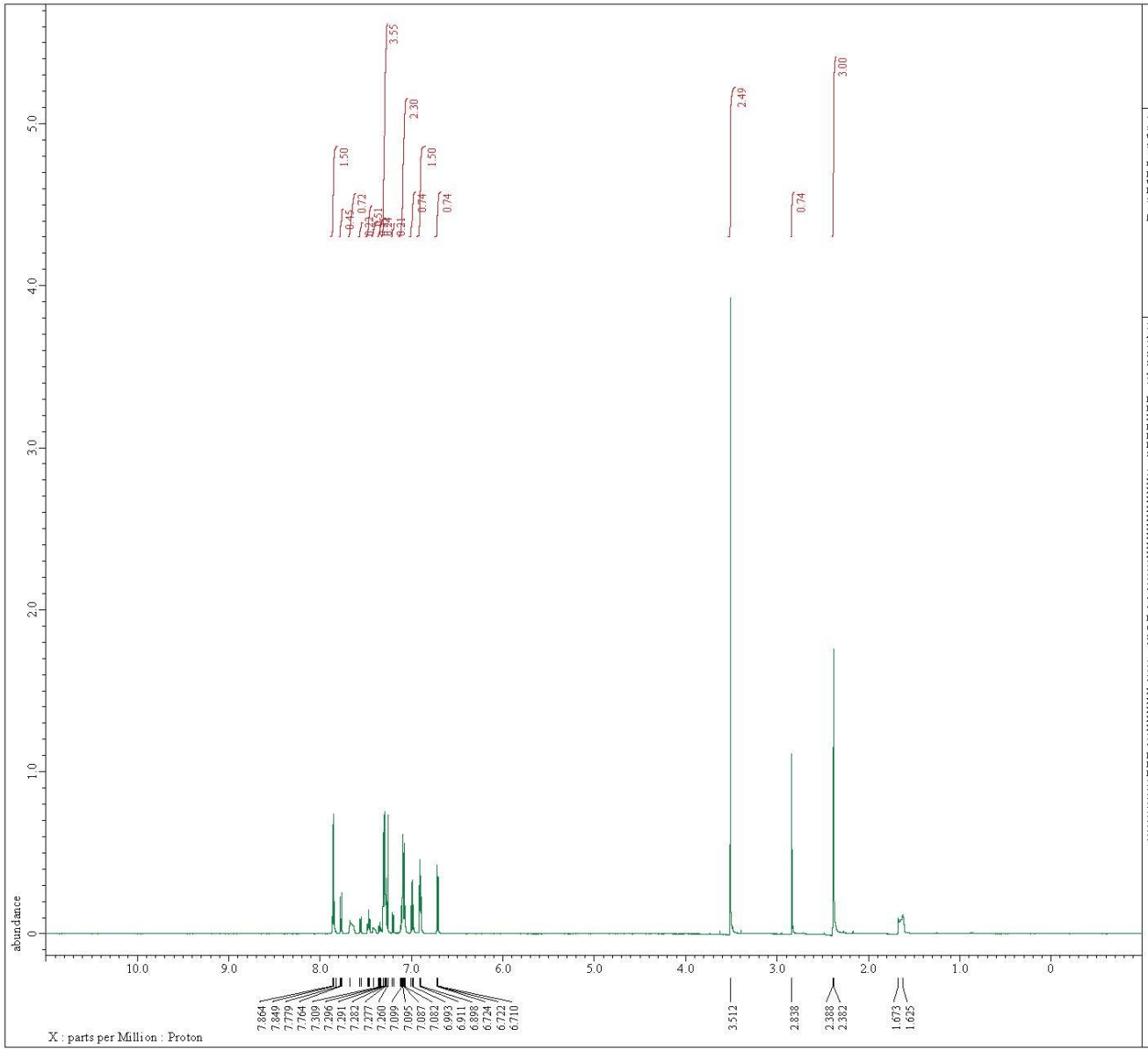


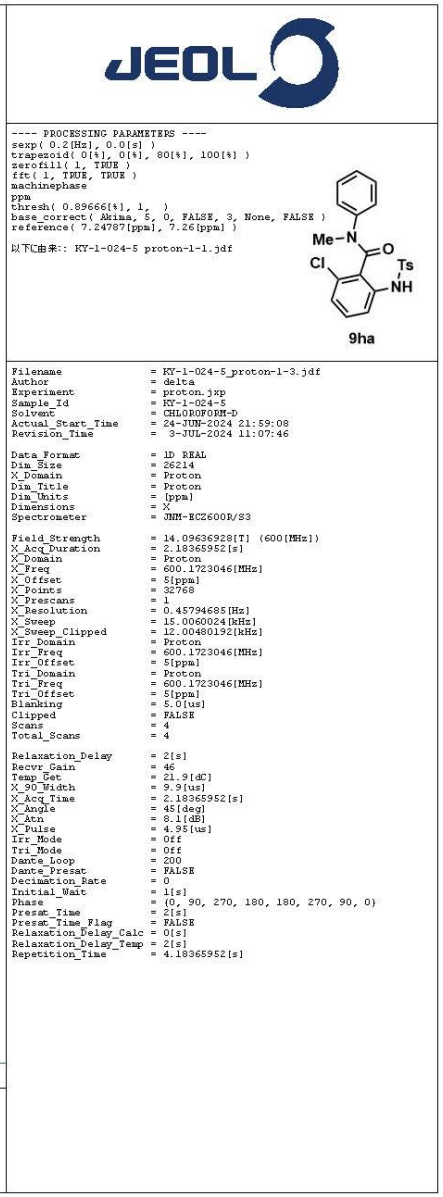

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

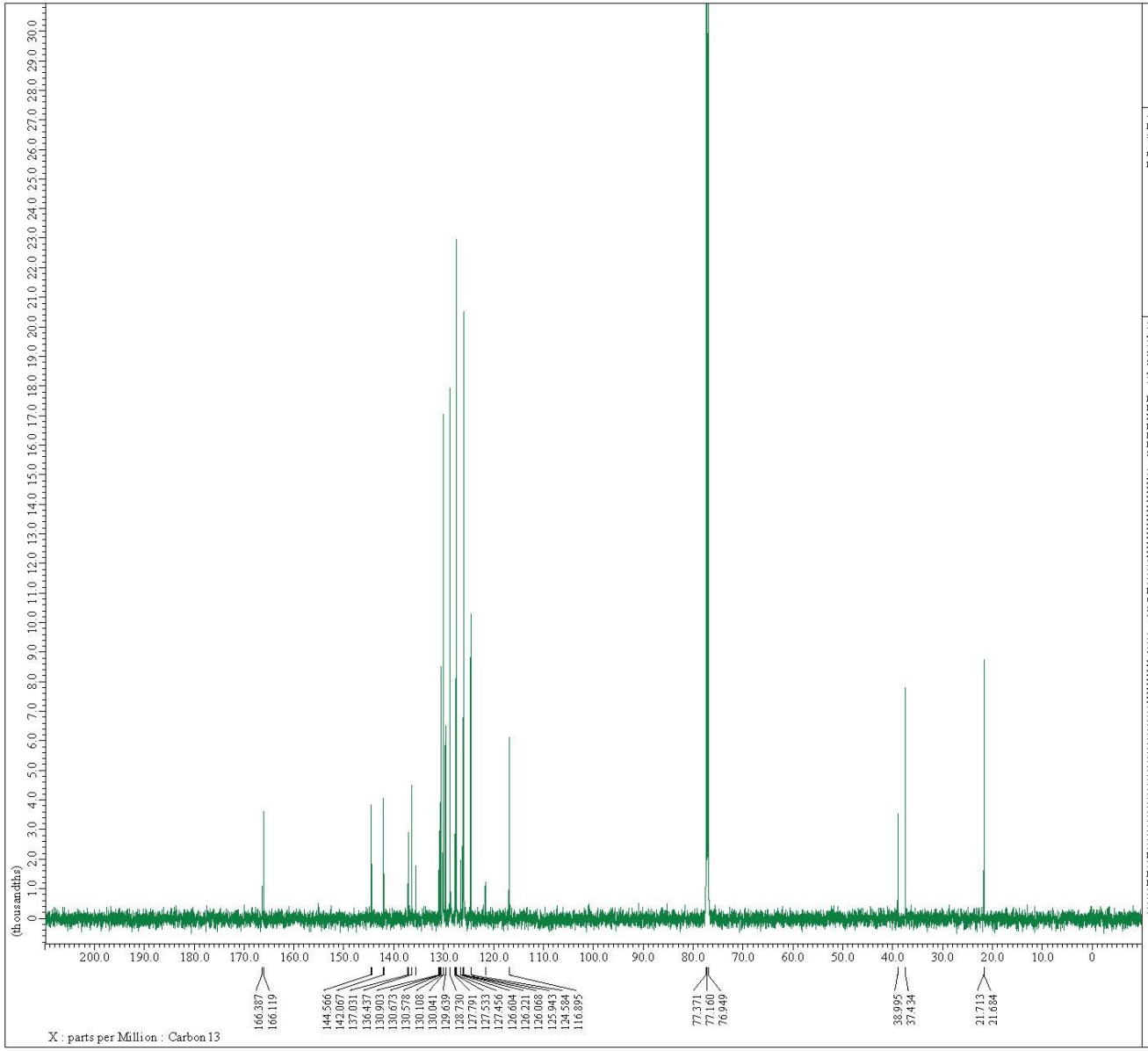
Filename	= KY-1-044-5_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= KY-1-044-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JUN-2024 12:47:06
Revision_Time	= 24-JUN-2024 08:13:07
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= 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	= 36
Temp_Set	= 22.1[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	= (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.18365952[s]

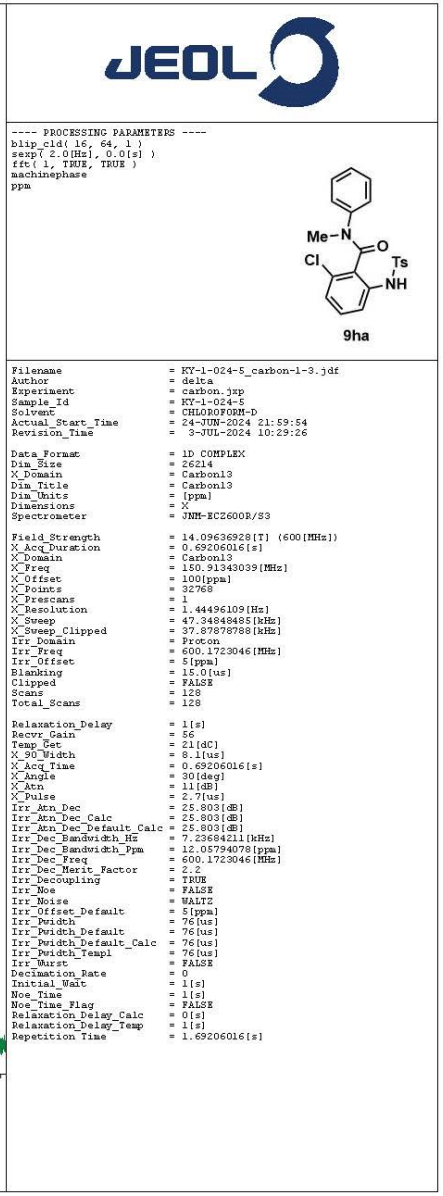

(thousandths)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
167.747
144.346
143.762
137.136
136.342
133.843
132.895
129.927
129.524
127.571
127.399
126.250
126.106
123.942
116.043
77.371
77.160
76.949
38.507
21.674
X : parts per Million : Carbon13

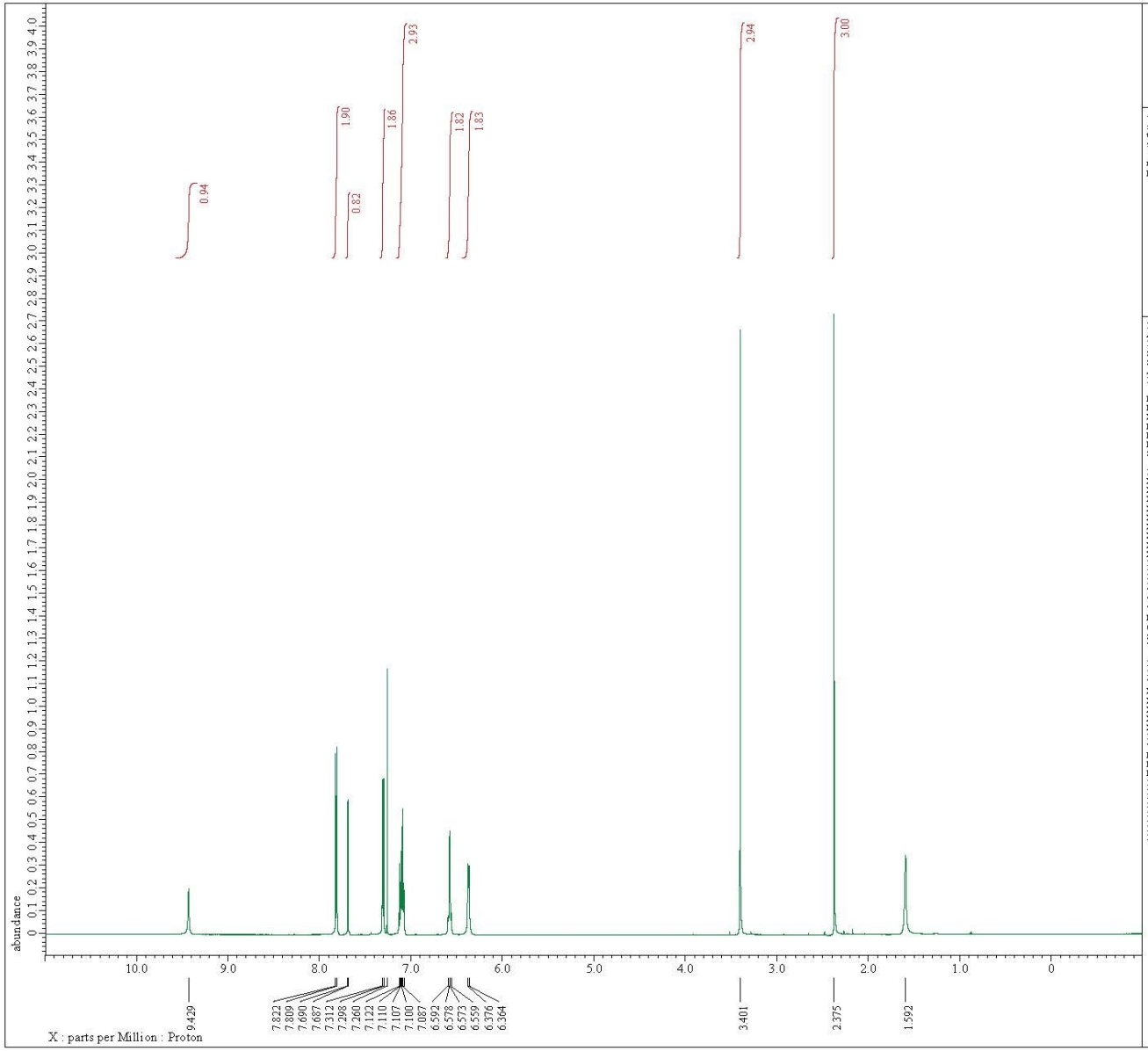

---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
Me–N
O
Ts
NH
Br
9ga
Filename = KY-1-044-5_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = KY-1-044-5
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-JUN-2024 12:49:07
Revision_Time = 23-JUN-2024 13:28:53
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 = 512
Total_Scans = 512
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 22[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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]


3.55
2.30
1.50
1.50
0.74
0.74
0.72
0.45
2.49
0.74
3.00
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.864
7.849
7.779
7.764
7.309
7.296
7.291
7.282
7.277
7.260
7.099
7.095
7.087
7.082
6.993
6.911
6.808
6.734
6.722
6.710
3.512
2.838
2.388
2.382
1.673
1.625
X : parts per Million : Proton

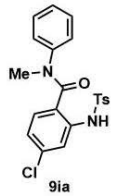

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(0.89666[%], 1,)
base_correct(Akima, 5, 0, FALSE, 3, None, FALSE)
reference(7.24787[ppm], 7.26[ppm])
以下由来:: KY-1-024-5 proton-1-1.jdf
Me
N
O
Cl
Ts
NH
9ha
Filename = KY-1-024-5_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = KY-1-024-5
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-JUN-2024 21:59:08
Revision_Time = 3-JUL-2024 11:07:46
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[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 = 46
Temp_Get = 21.9[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 = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
RelaxationDelay_Calc = 0[s]
RelaxationDelay_Temp = 2[s]
Repetition_Time = 4.18365952[s]


(thousandths)
X : parts per Million : Carbon13
166.387
166.119
144.566
142.067
137.031
136.437
130.903
130.673
130.578
130.108
130.041
129.639
128.730
127.791
127.533
127.456
126.604
126.221
126.068
125.943
124.584
116.895
77.371
77.160
76.949
38.995
37.434
21.713
21.684


---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
Me
N
O
Cl
Ts
NH
9ha
Filename = KY-1-024-5_carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = KY-1-024-5
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-JUN-2024 21:59:54
Revision_Time = 3-JUL-2024 10:29:26
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 = 128
Total_Scans = 128
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 21[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_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = FALSE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Declination_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]

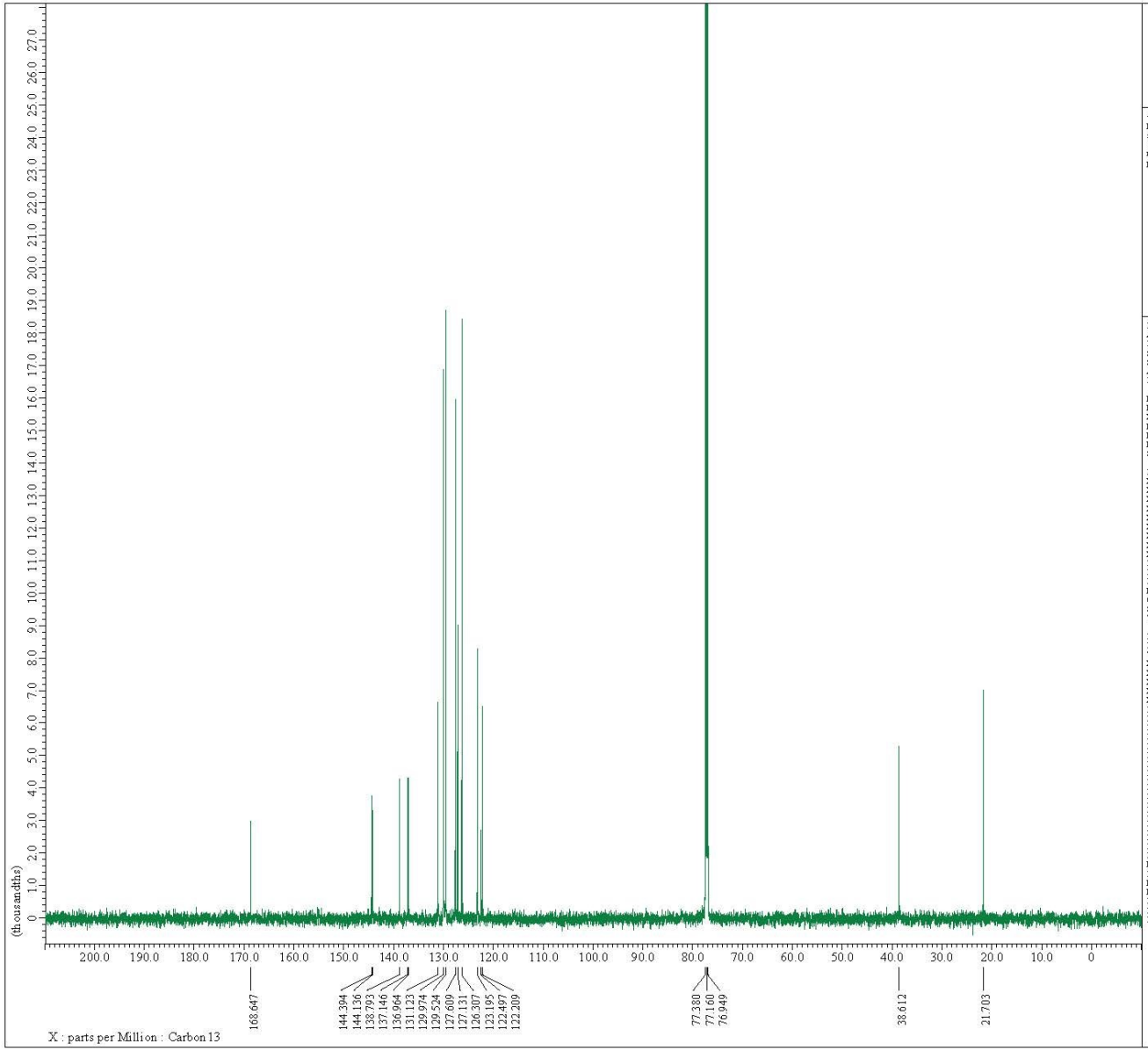


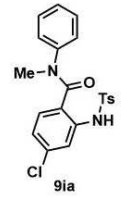
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm



9ia

Filename	= KY-1-047-5_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= KY-1-047-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JUN-2024 13:10:23
Revision_Time	= 3-JUL-2024 11:14:51
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	= 46
Temp_Set	= 21.4[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	= (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.18365952[s]

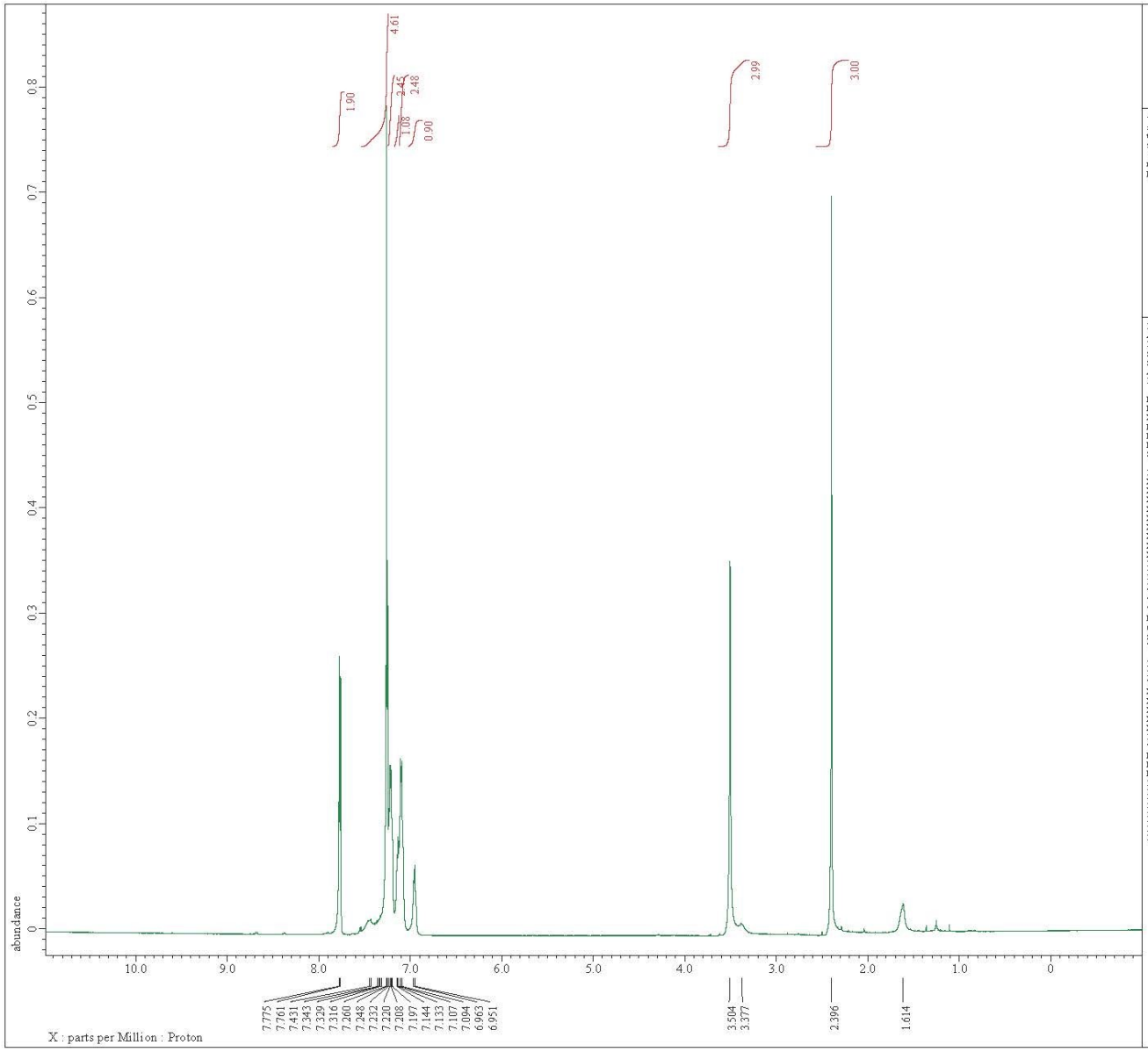


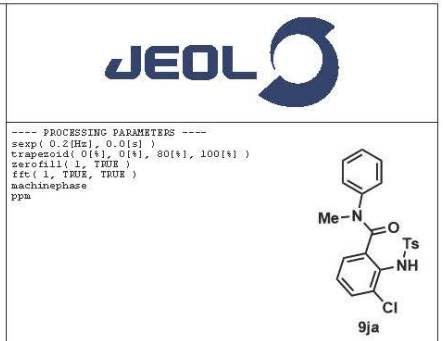


9ia

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

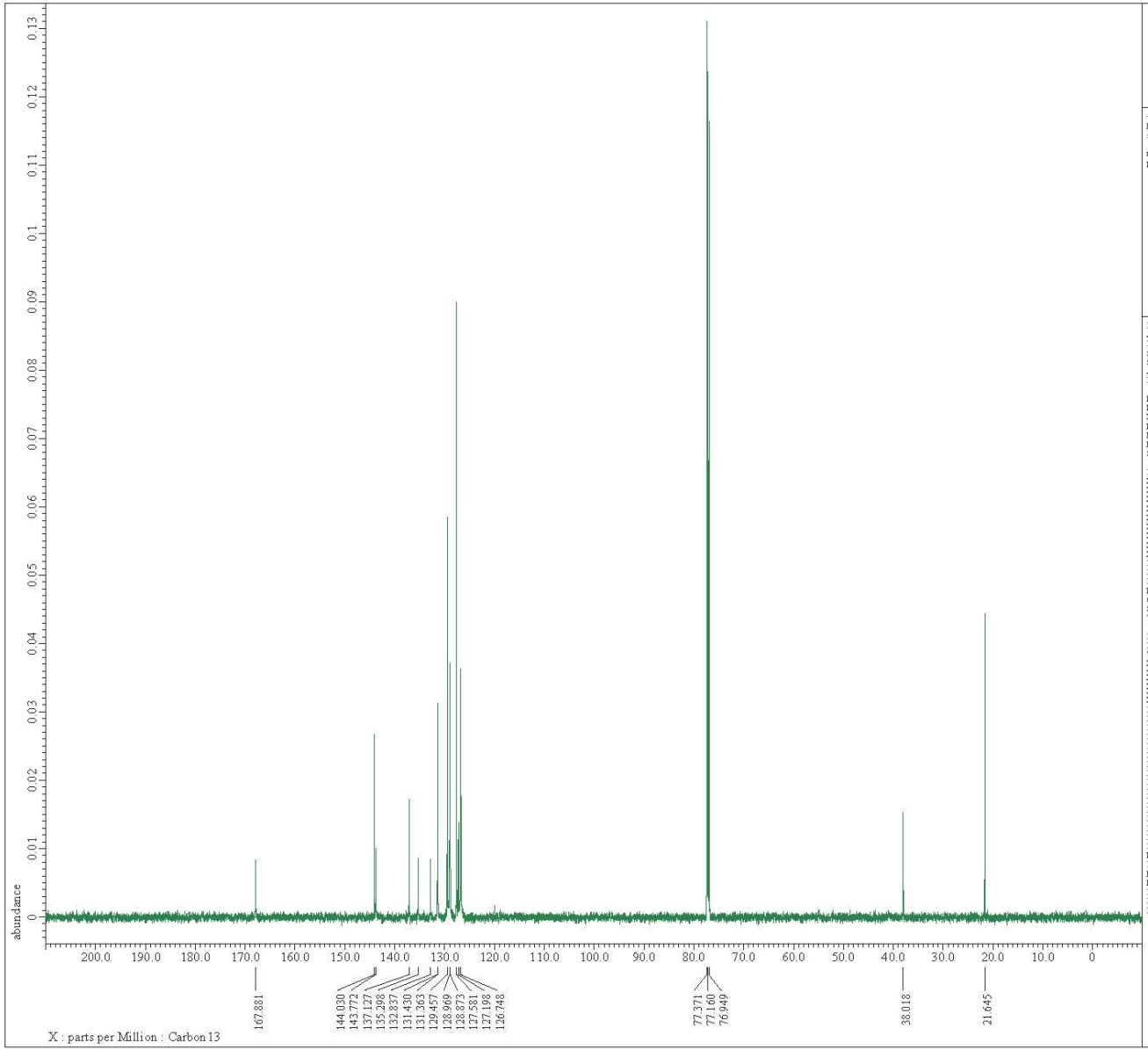
Filename	= KY-1-047-5_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-1-047-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JUN-2024 13:12:23
Revision_Time	= 23-JUN-2024 13:31:28
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 256
Total_Scans	= 256
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21.3[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_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

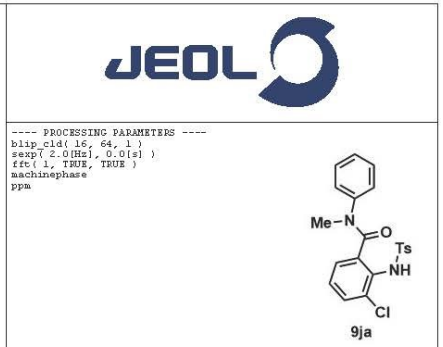





```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= TK-6-151-2-1_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-6-151-2-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-JUN-2024 22:44:36
Revision_Time	= 27-JUN-2024 08:02:01
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	= 2.91110912[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.34351169[Hz]
X_Sweep	= 11.2561909[kHz]
X_Sweep_Clipped	= 9.00498272[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	= 46
Temp_Get	= 20.9[dC]
X_90_Width	= 9.9[us]
X_Acq_Time	= 2.91110912[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	= {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.91110912[s]

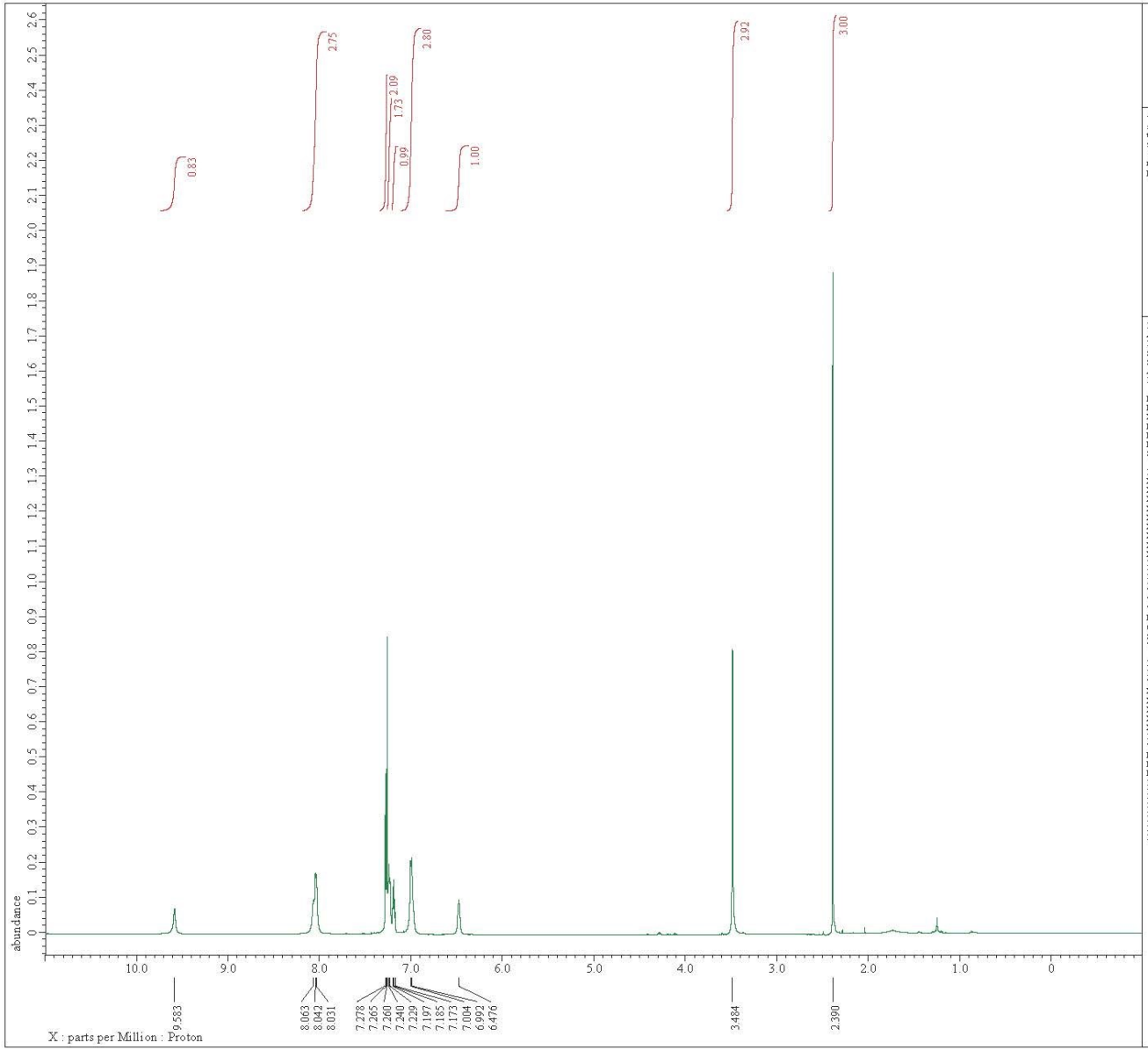





```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

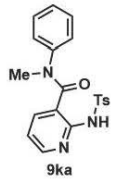

9ja

Filename	= TK-6-151-2-2_carbon-1-3.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-151-2-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-JUN-2024 22:40:37
Revision_Time	= 27-JUN-2024 08:05:02
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	= 32
Total_Scans	= 32
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_Default_Calc	= 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_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



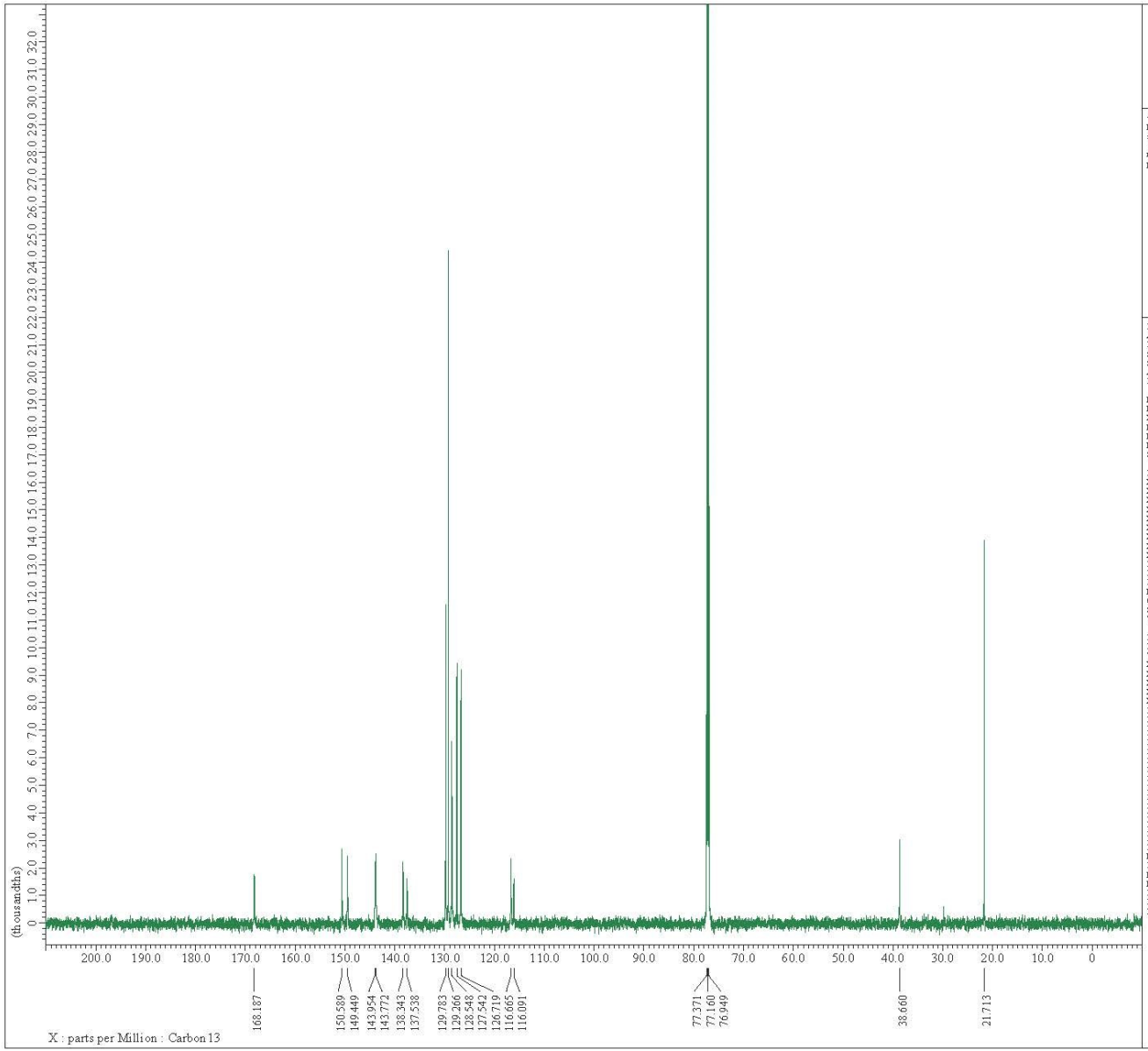
JEOL

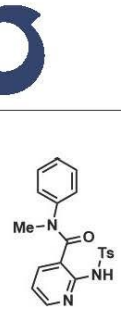
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```



9ka

```
Filename                = TK-6-149-3_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-149-3
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 25-JUN-2024 21:28:19
Revision_Time           = 26-JUN-2024 08:53:53

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              = 36
Temp_Set                = 21.1[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```

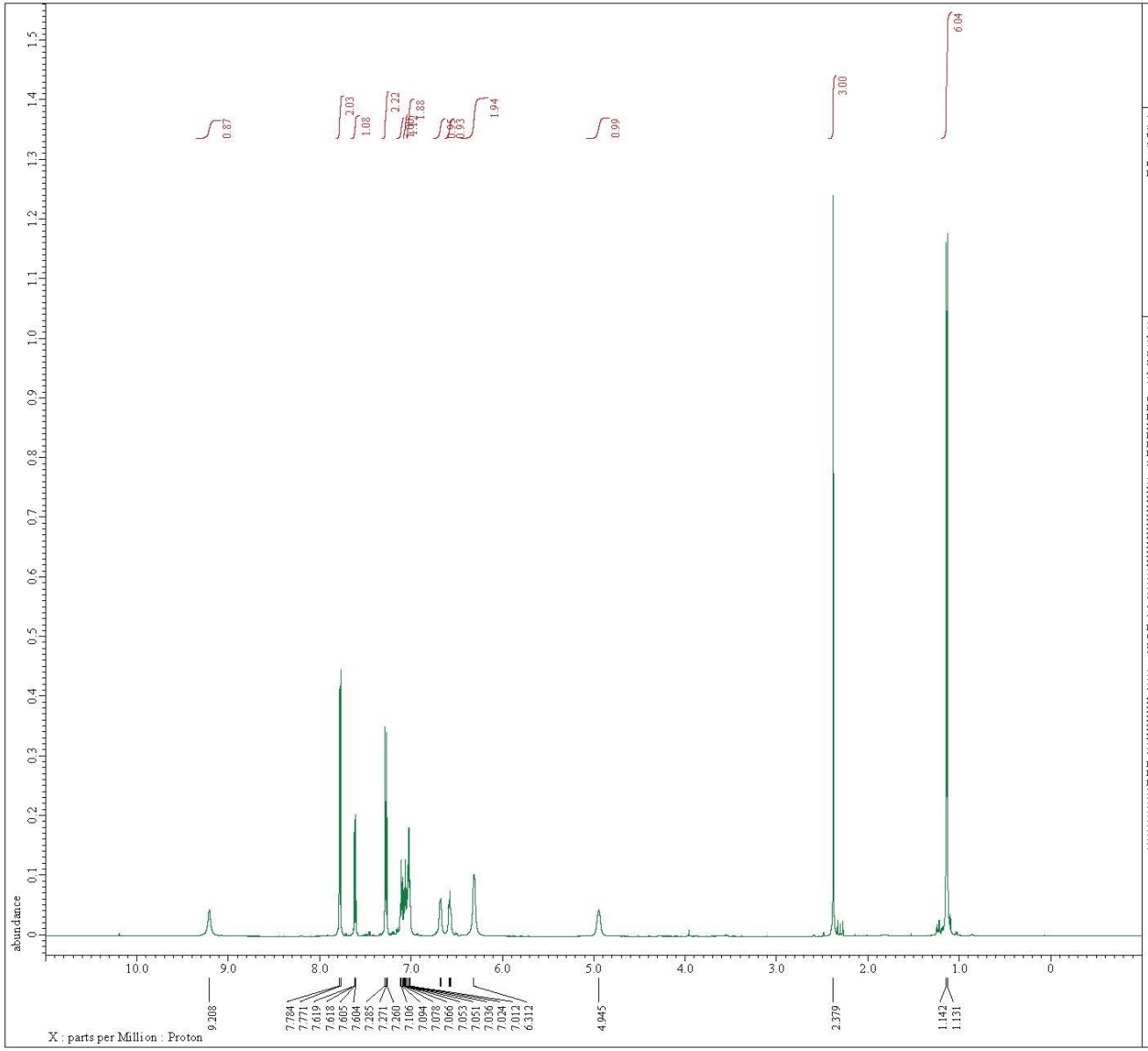


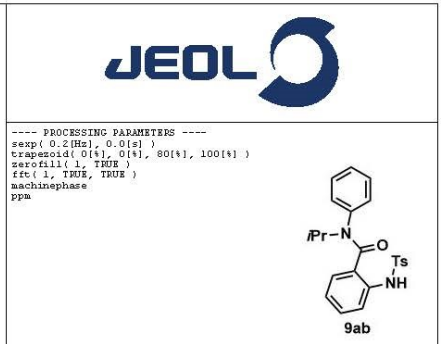


9ka

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

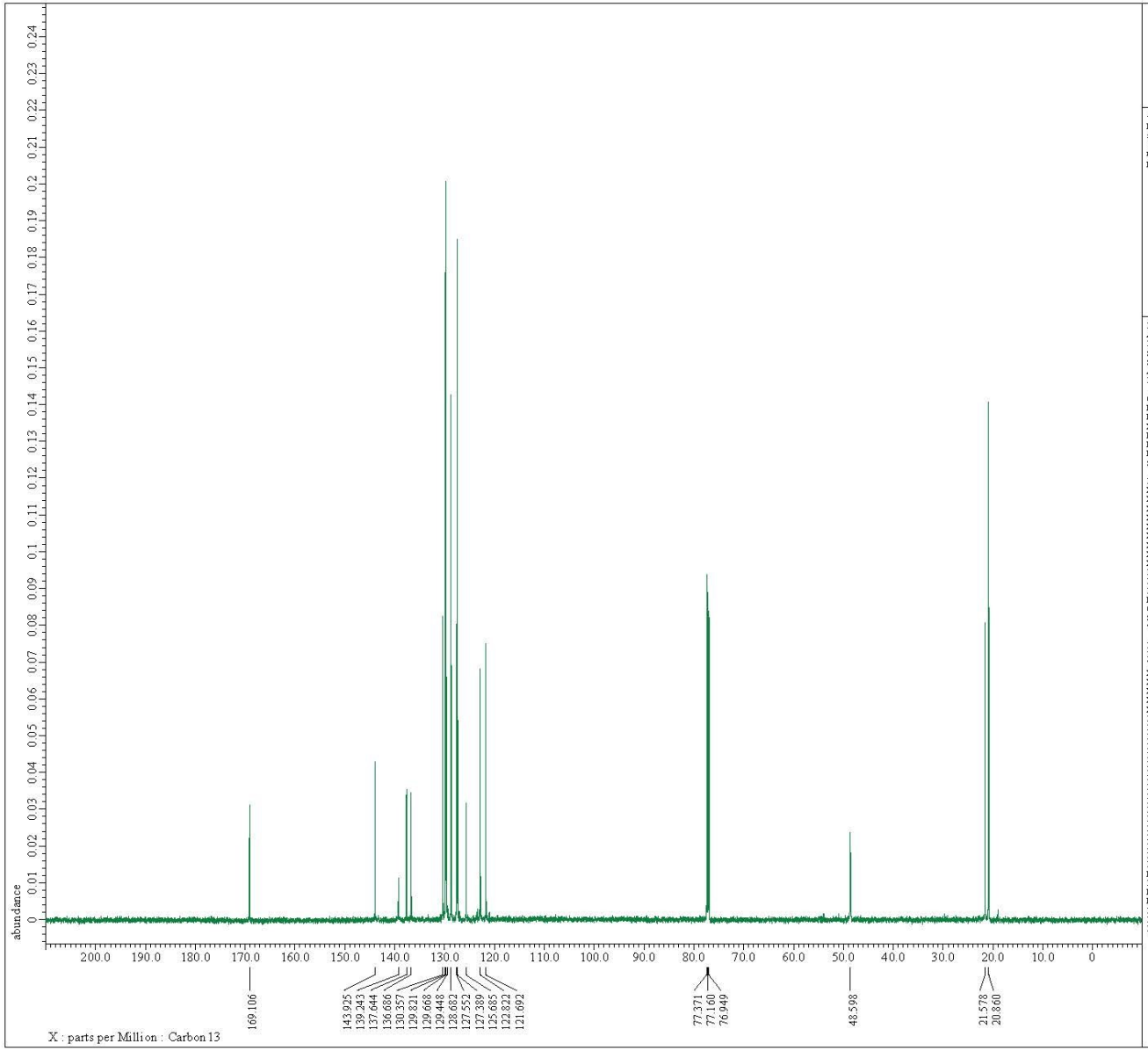
Filename	= TK-6-149-3_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-149-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2024 21:30:19
Revision_Time	= 25-JUN-2024 21:36:27
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 256
Total_Scans	= 256
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 21.3[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]





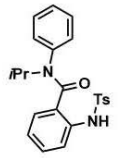

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= KY-1-033-1_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= KY-1-033-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-APR-2024 10:42:29
Revision_Time	= 24-APR-2024 14:35:58
Comment	= single_pulse
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	= 10[s]
Recvr_Gain	= 26
Temp_Get	= 22.5[dC]
X_90_Width	= 9.9[us]
X_Acq_Time	= 2.90455552[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 1000
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time	= 10[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 10[s]
Repetition_Time	= 12.90455552[s]



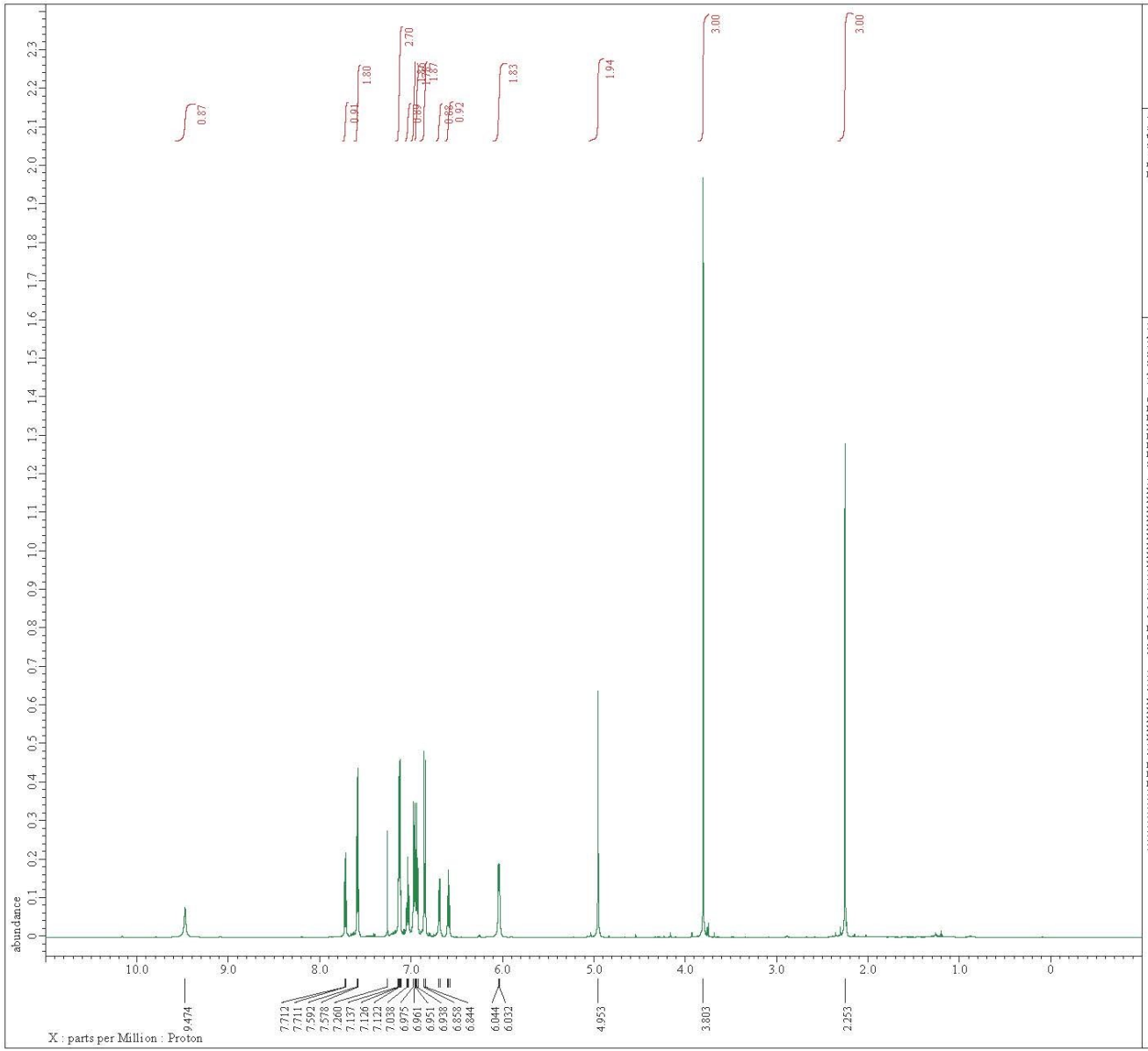
JEOL

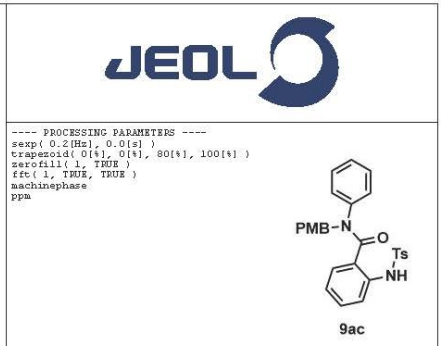
```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```



9ab

Filename	= KY-1-033-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-1-033-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-APR-2024 10:44:08
Revision_Time	= 24-APR-2024 10:45:59
Comment	= single pulse decoupled gated NOE
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	= 33
Total_Scans	= 33
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 22.5[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_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

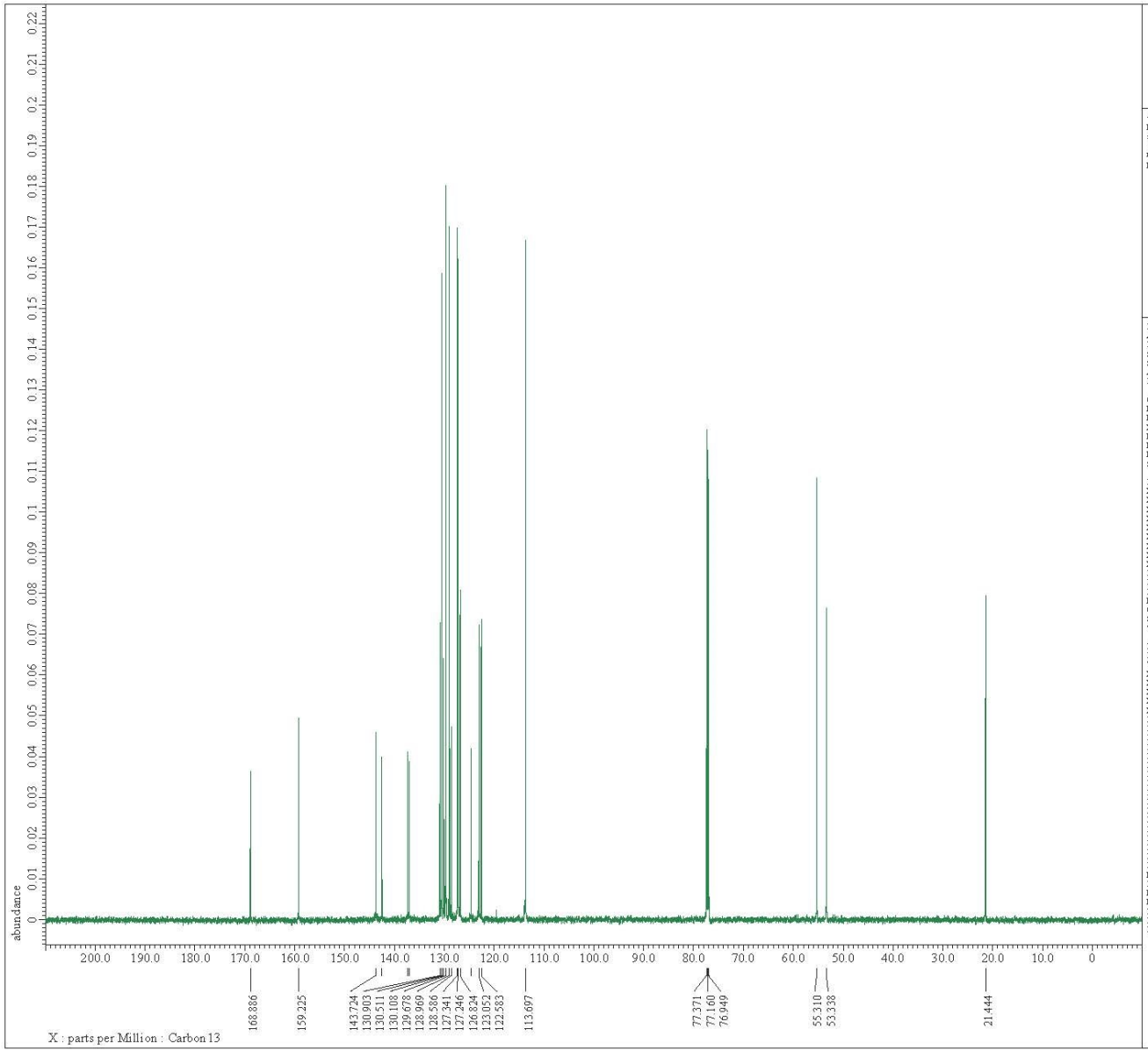


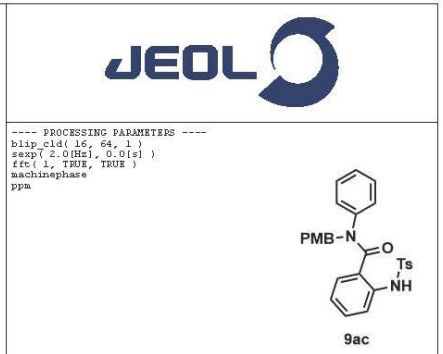



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```


9ac

```
Filename                = KY-1-032-1_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = KY-1-032-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 24-APR-2024 10:35:09
Revision_Time           = 24-APR-2024 14:52:40

Comment                 = single_pulse
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        = 10[s]
Recvr_Gain              = 26
Temp_Get                = 22.5[dC]
X_90_Width              = 9.9[us]
X_Acq_Time              = 2.90455552[s]
X_Angle                 = 45[deg]
X_Atn                   = 8.1[dB]
X_Pulse                 = 4.95[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 1000
Dante_Presat            = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 10[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 10[s]
Repetition_Time         = 12.90455552[s]
```

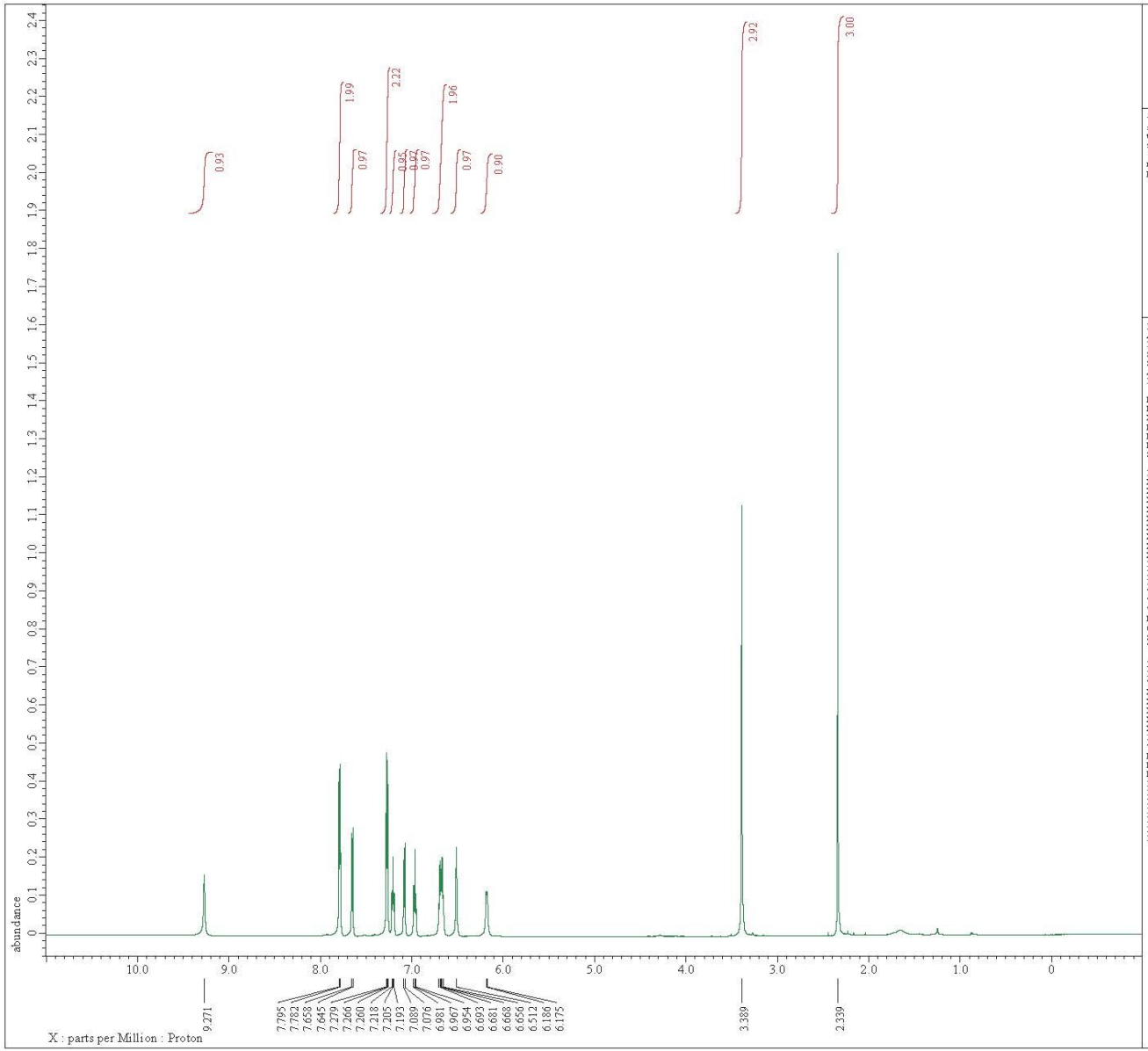


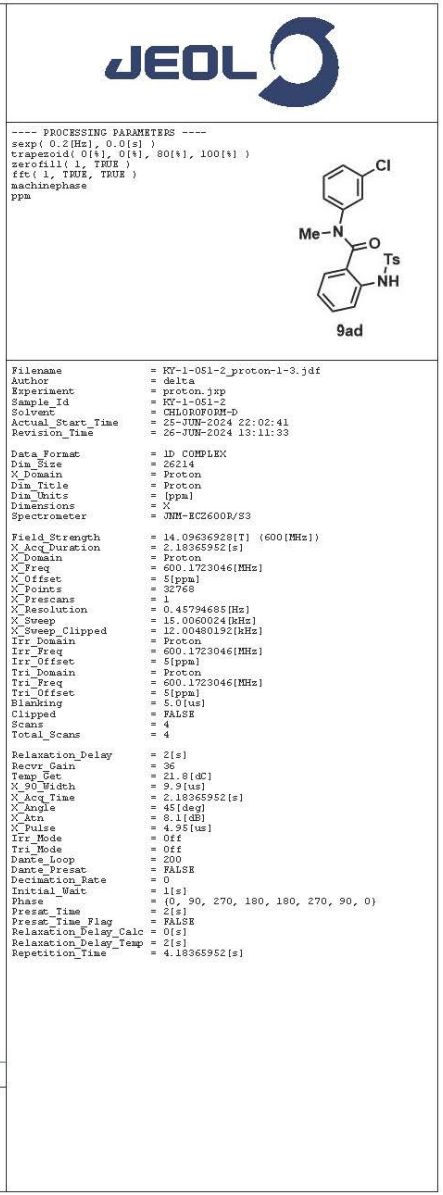


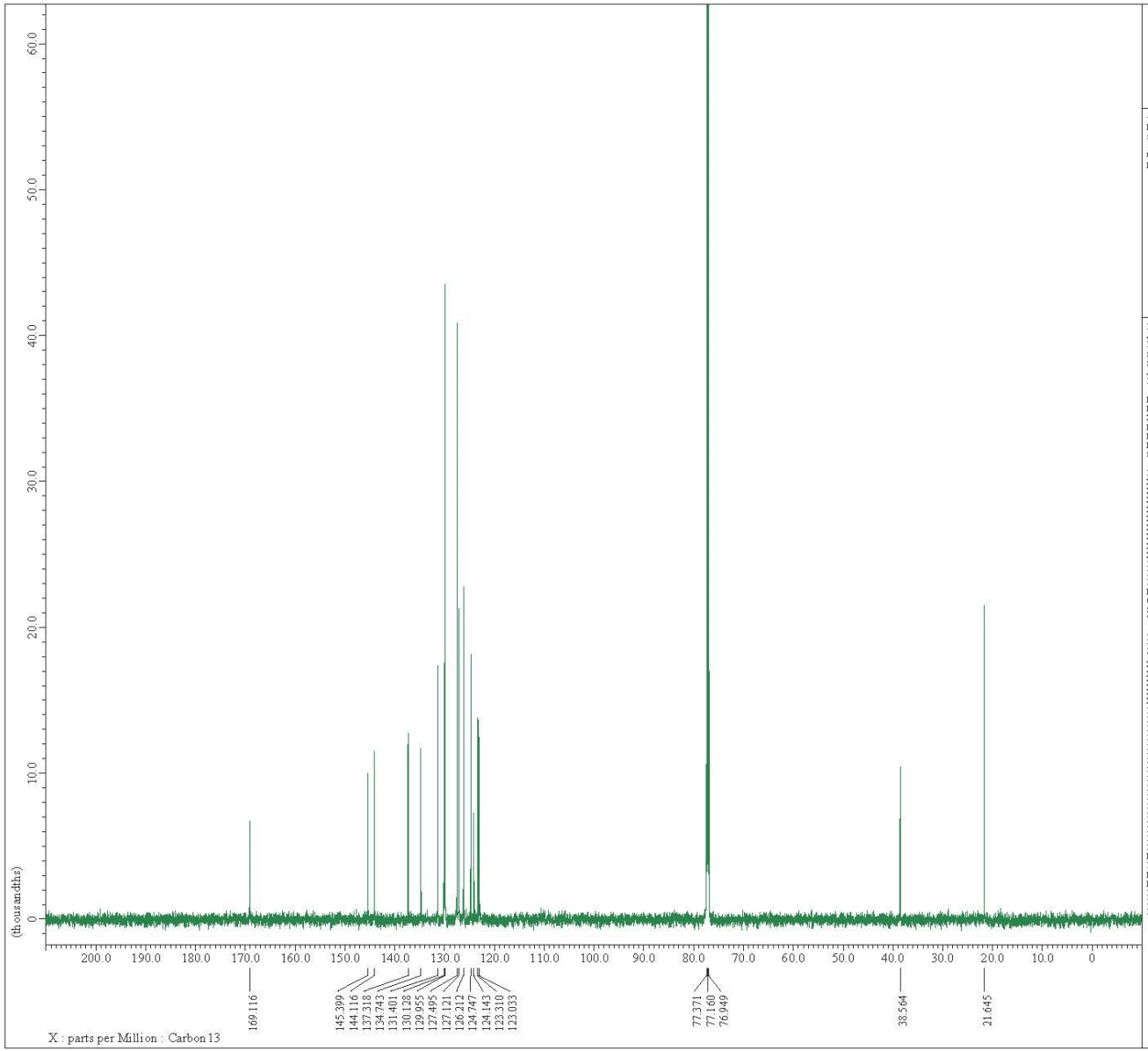

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
ffc( 1, TRUE, TRUE )
machinephase
ppm
```


9ac

Filename	= KY-1-032-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-1-032-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-APR-2024 10:36:47
Revision_Time	= 24-APR-2024 10:38:56
Comment	= single pulse decoupled gated NOE
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	= 39
Total_Scans	= 39
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 22.5[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_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

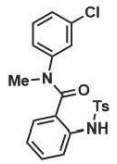

abundance
X : parts per Million : Proton
0.93
1.99
0.97
2.22
0.95
0.92
0.97
1.96
0.97
0.90
2.92
3.00
9.271
7.795
7.782
7.658
7.645
7.279
7.266
7.260
7.218
7.205
7.193
7.089
7.076
6.981
6.967
6.954
6.693
6.681
6.668
6.656
6.512
6.186
6.175
3.389
2.339


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Cl
Me–N
O
Ts
NH
9ad
Filename = KY-1-051-2_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = KY-1-051-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-JUN-2024 22:02:41
Revision_Time = 26-JUN-2024 13:11:33
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 = 36
Temp_Get = 21.8[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 = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18365952[s]



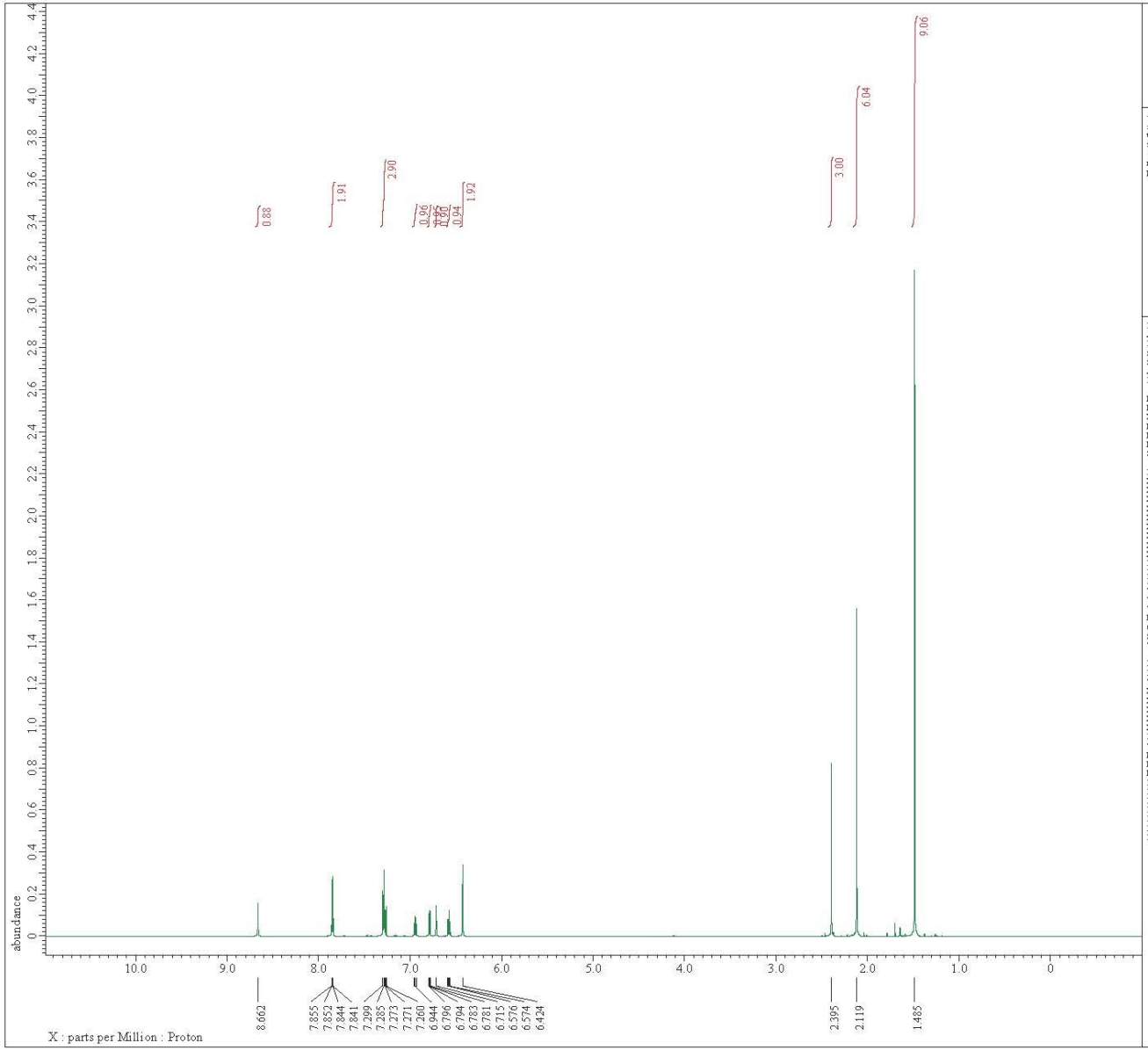
JEOL

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



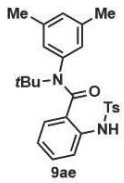
9ad

Filename	= KY-1-051-2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY-1-051-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2024 22:04:42
Revision_Time	= 25-JUN-2024 22:04:20
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[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	= 64
Total_Scans	= 64
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

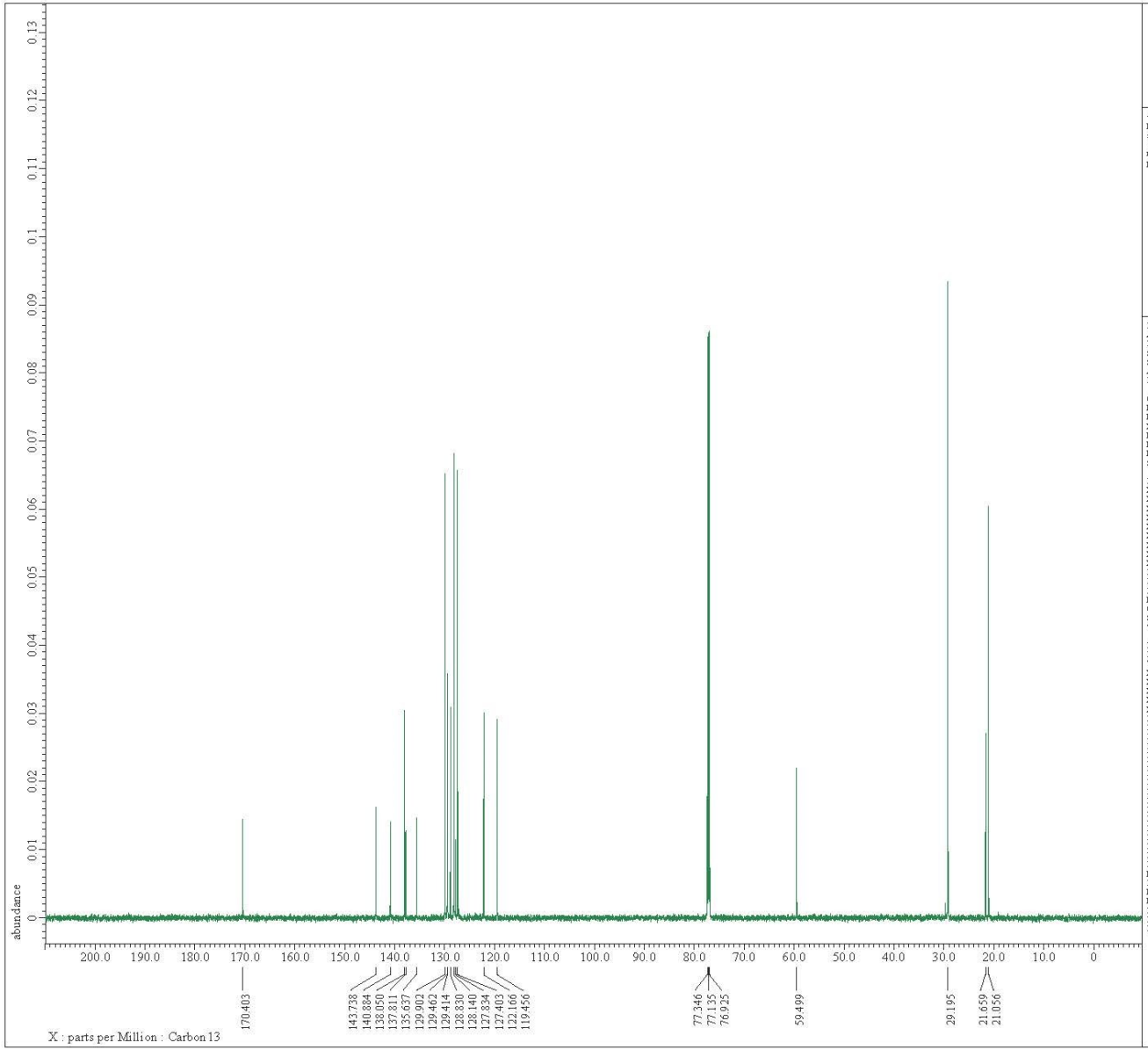


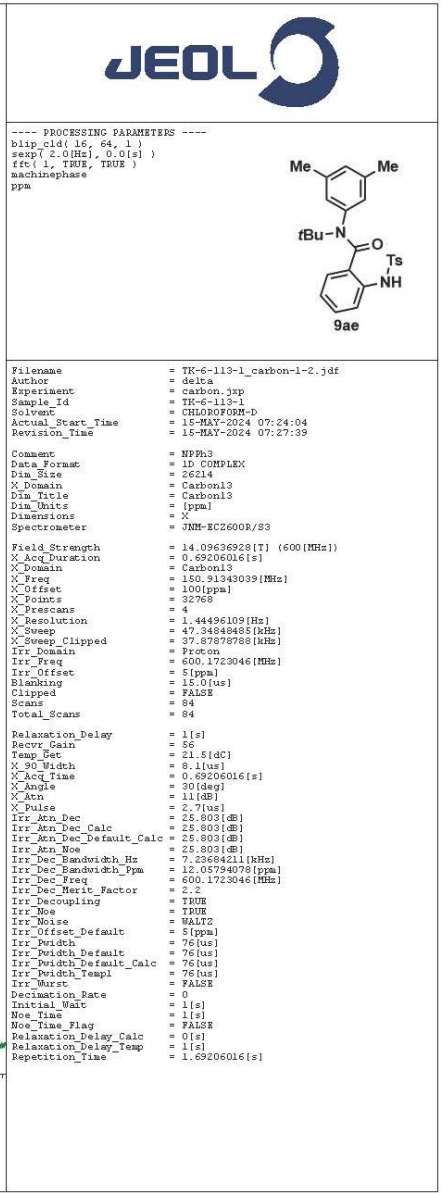
JEOL

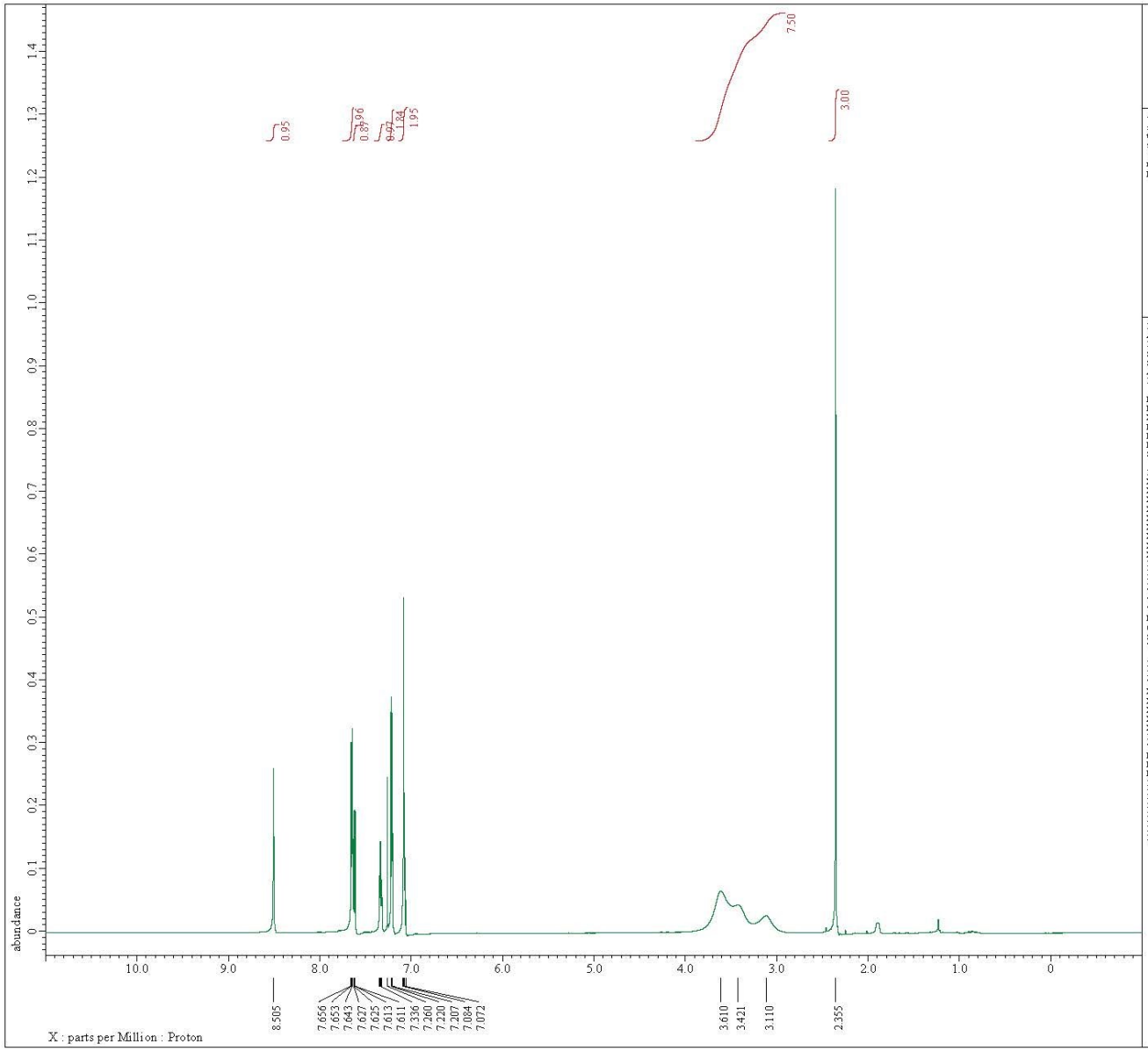
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```




```
Filename                = TK-6-113-1_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-113-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 15-MAY-2024 07:23:10
Revision_Time           =  4-JUL-2024 21:23:08

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[MHz])
X_Acq_Duration          = 2.18103808[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                   = 4
Total_Scans             = 4

Relaxation_Delay        = 2[s]
Recvr_Gain              = 26
Temp_Set                = 21.5[dC]
X_90_Width              = 9.9[us]
X_Acq_Time              = 2.18103808[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18103808[s]
```

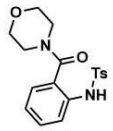

abundance
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.403
143.738
140.884
138.050
137.811
135.637
129.902
129.462
129.414
128.830
128.140
127.834
127.403
122.166
119.456
77.346
77.135
76.925
59.499
29.195
21.659
21.056
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
Me
Me
tBu-N
O
Ts
NH
9ae
Filename = TK-6-113-1_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-113-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-MAY-2024 07:24:04
Revision_Time = 15-MAY-2024 07:27:39
Comment = NPPh3
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 = 84
Total_Scans = 84
Relaxation_Delay = 1[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_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]



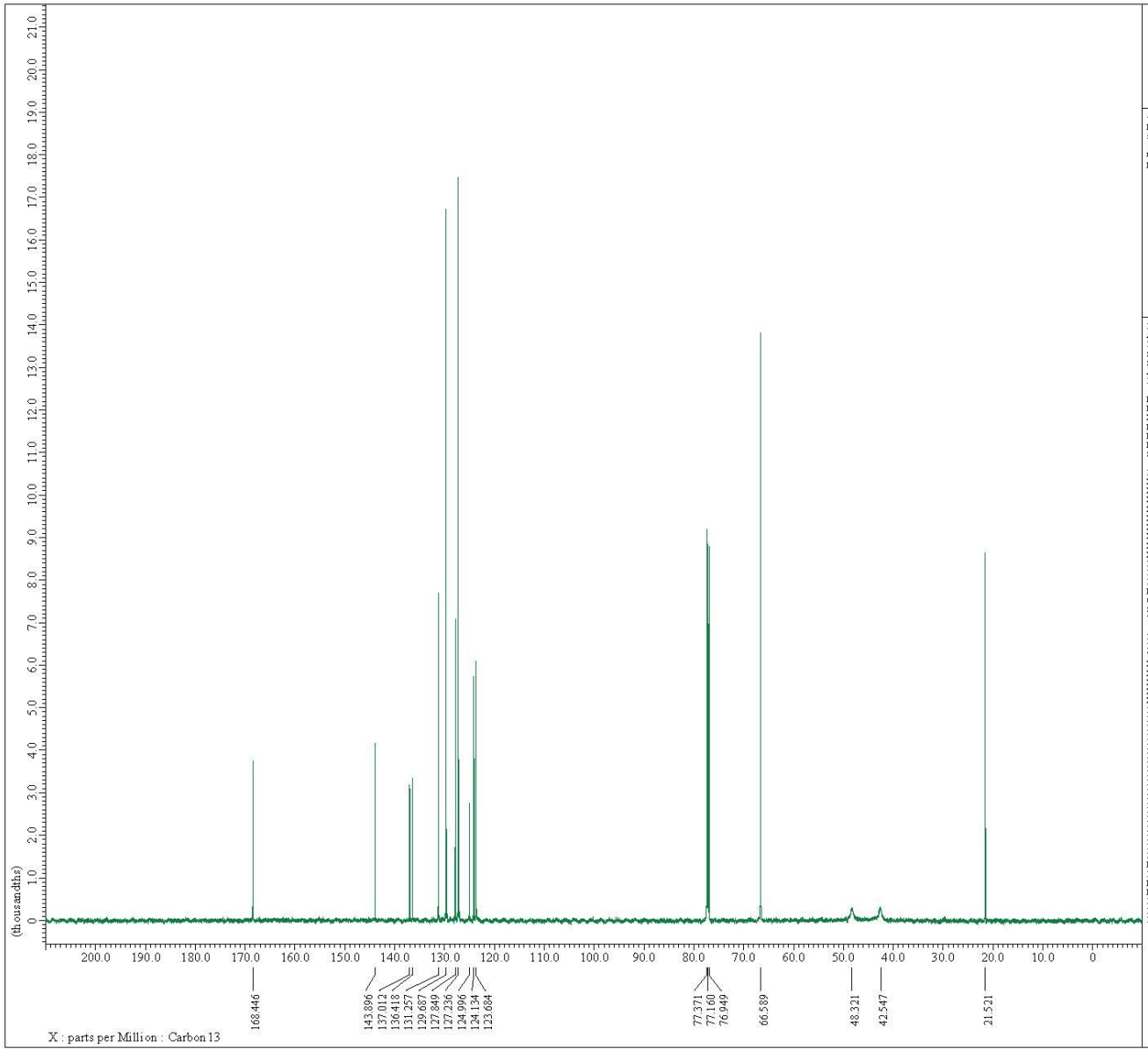
JEOL

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



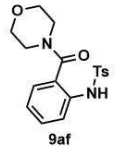
9af

```
Filename                = TK-6-072-2_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-072-2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 13-APR-2024 09:41:58
Revision_Time           = 13-APR-2024 11:52:42

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                = 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                   = 4
Total_Scans             = 4

Relaxation_Delay        = 1[s]
Recvr_Gain              = 26
Temp_Get                = 21.7[dC]
X_90_Width              = 9.9[us]
X_Acq_Time              = 2.18103808[s]
X_Angle                 = 45[deg]
X_Atn                   = 8.1[dB]
X_Pulse                 = 4.95[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 100
Dante_Presat            = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 1[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 1[s]
Repetition_Time         = 3.18103808[s]
```



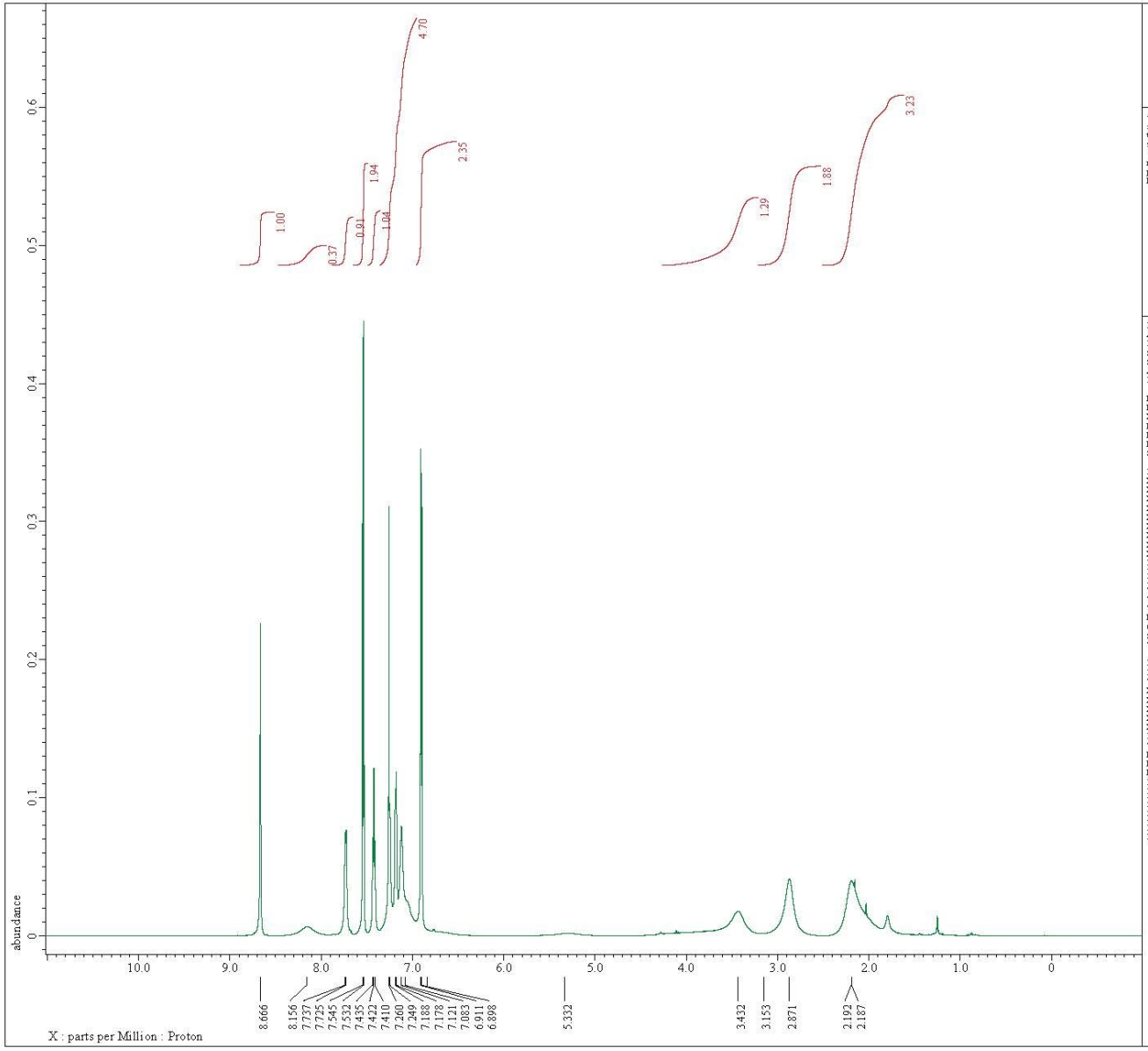
JEOL

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



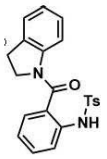
9af

Filename	= TK-6-072-2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-072-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-APR-2024 09:42:50
Revision_Time	= 13-APR-2024 09:47:08
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	= TRUE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Set	= 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	= 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 2.69206016[s]



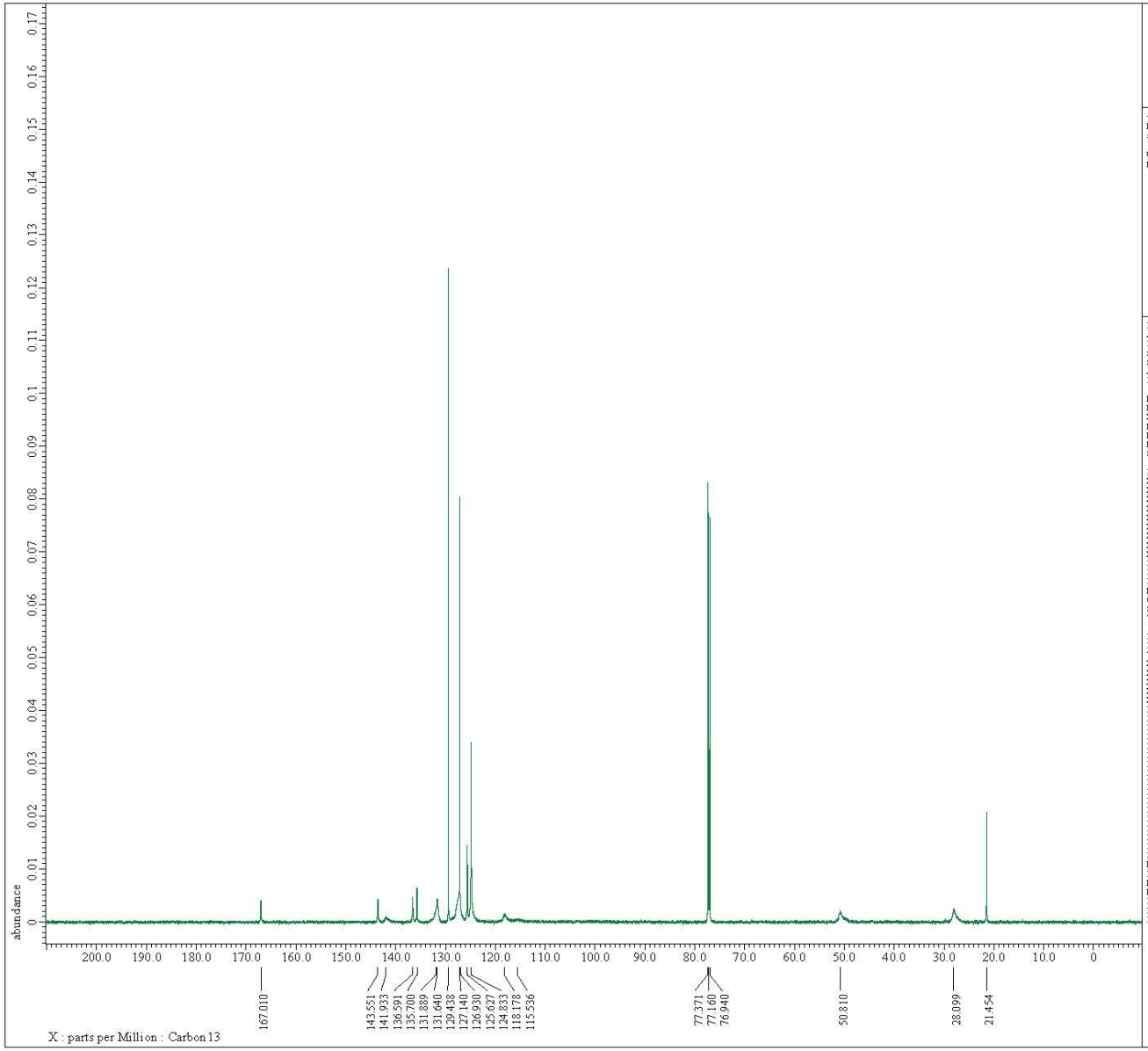
JEOL

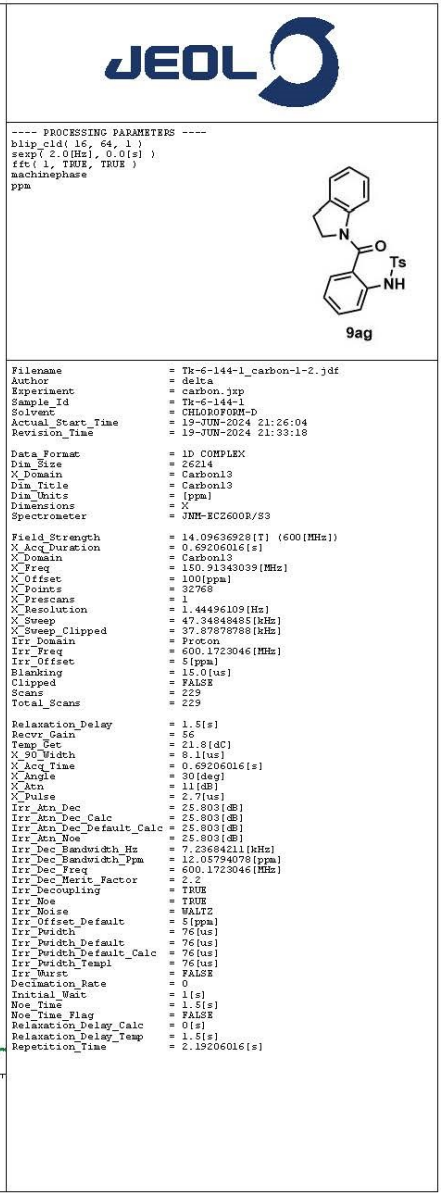
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FALSE )
```

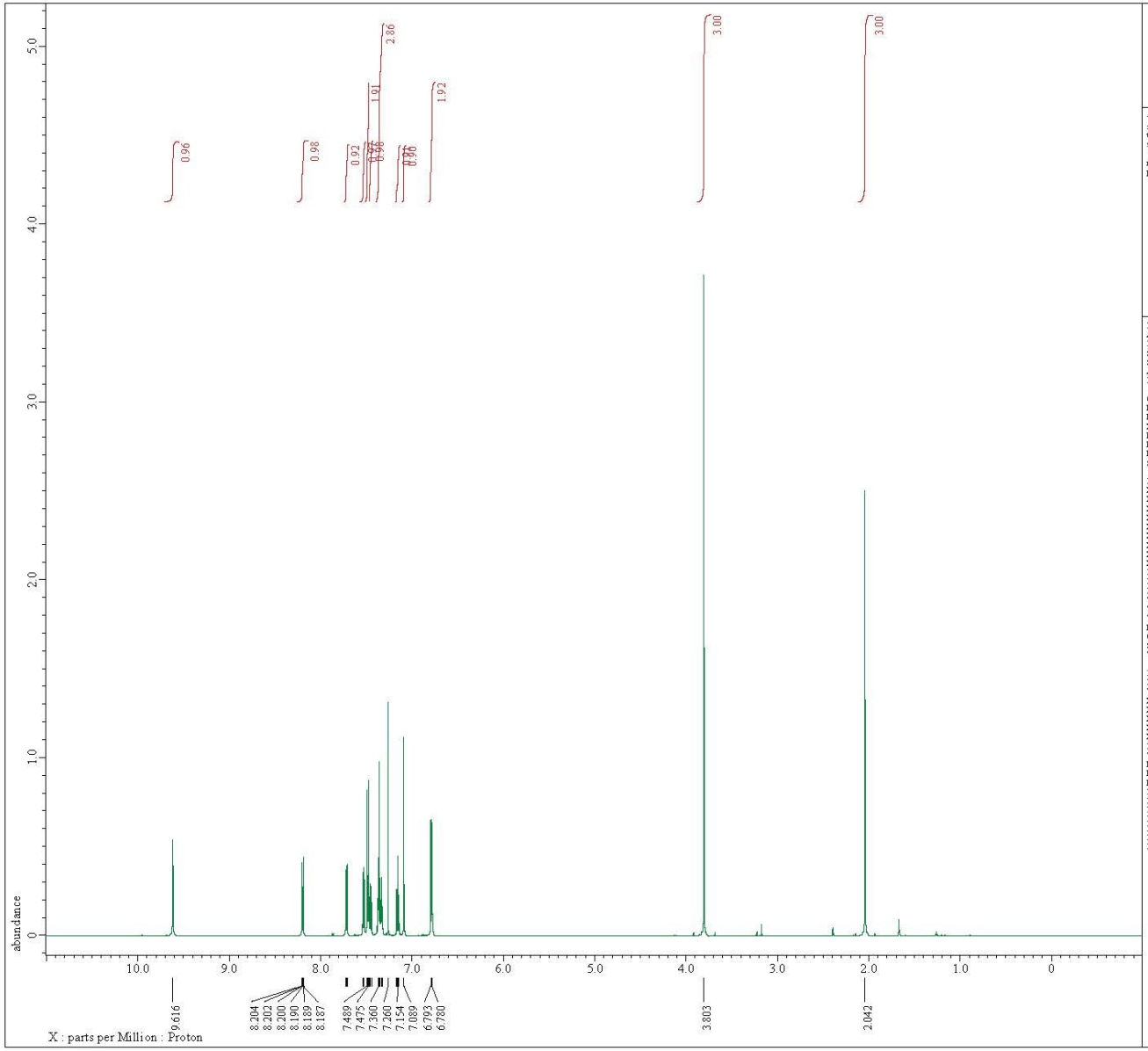


9ag

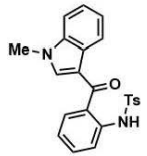
```
Filename                = Tk-6-144-1_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = Tk-6-144-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 19-JUN-2024 21:24:04
Revision_Time           =  4-JUL-2024 21:31:54

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[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                = 20.8[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```


abundance
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
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
167.010
143.551
141.933
136.591
135.700
131.889
131.640
129.438
127.140
126.930
125.627
124.853
118.178
115.536
77.371
77.160
76.940
50.810
28.099
21.454
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
Ts
NH
O
N
9ag
Filename = Tk-6-144-1_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Tk-6-144-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2024 21:26:04
Revision_Time = 19-JUN-2024 21:33:18
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 = 229
Total_Scans = 229
Relaxation_Delay = 1.5[s]
Recvr_Gain = 56
Temp_Get = 21.8[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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1.5[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1.5[s]
Repetition_Time = 2.19206016[s]

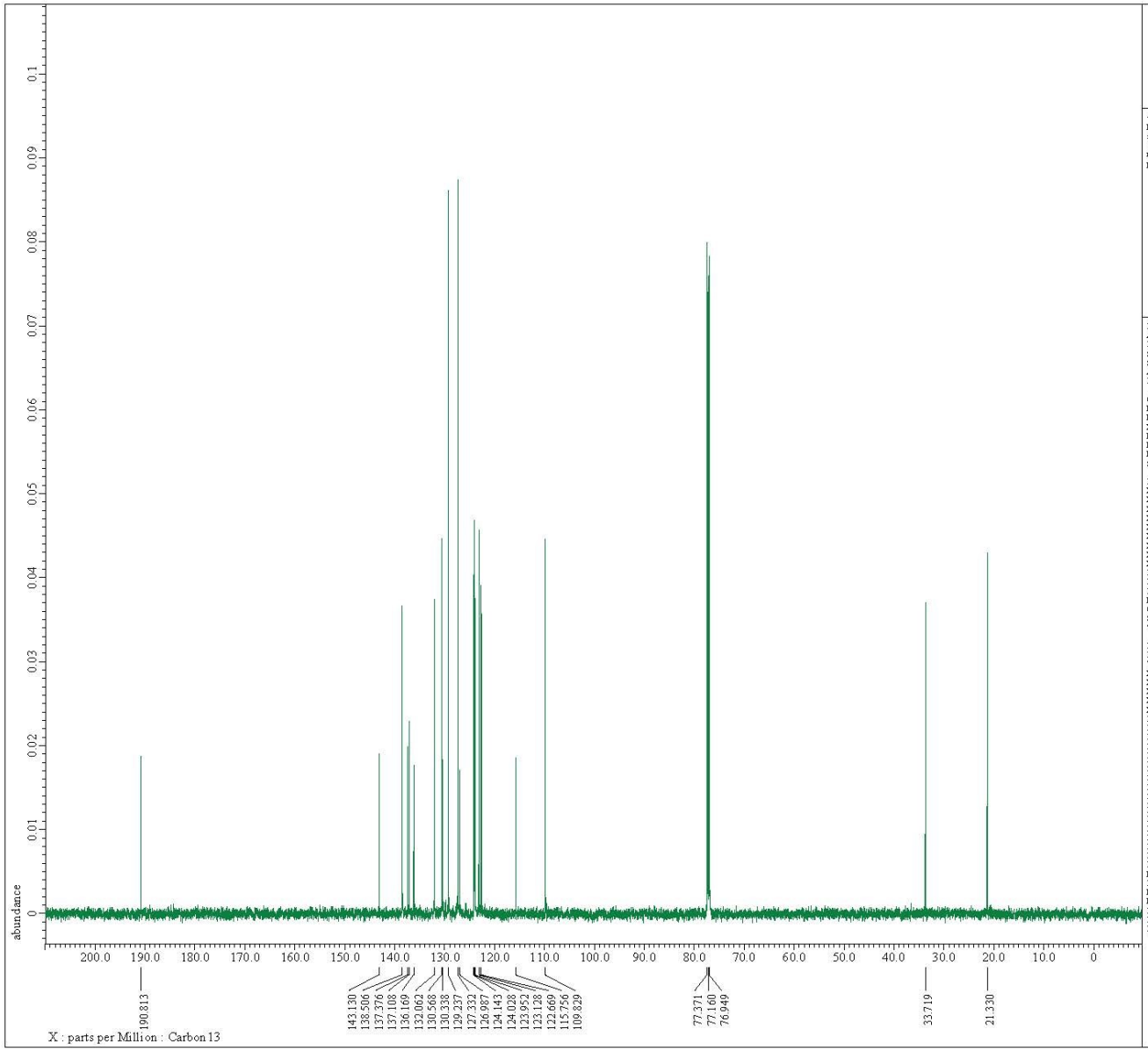


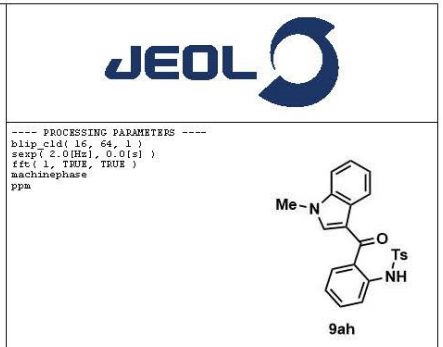
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm



9ah

Filename	= Tk-6-085-3_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= Tk-6-085-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-APR-2024 15:20:25
Revision_Time	= 1-JUL-2024 11:11:23
Comment	= single_pulse
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	= 10[s]
Recvr_Gain	= 36
Temp_Get	= 21.5[dC]
X_90_Width	= 9.9[us]
X_Acq_Time	= 2.90455552[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 1000
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time	= 10[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 10[s]
Repetition_Time	= 12.90455552[s]

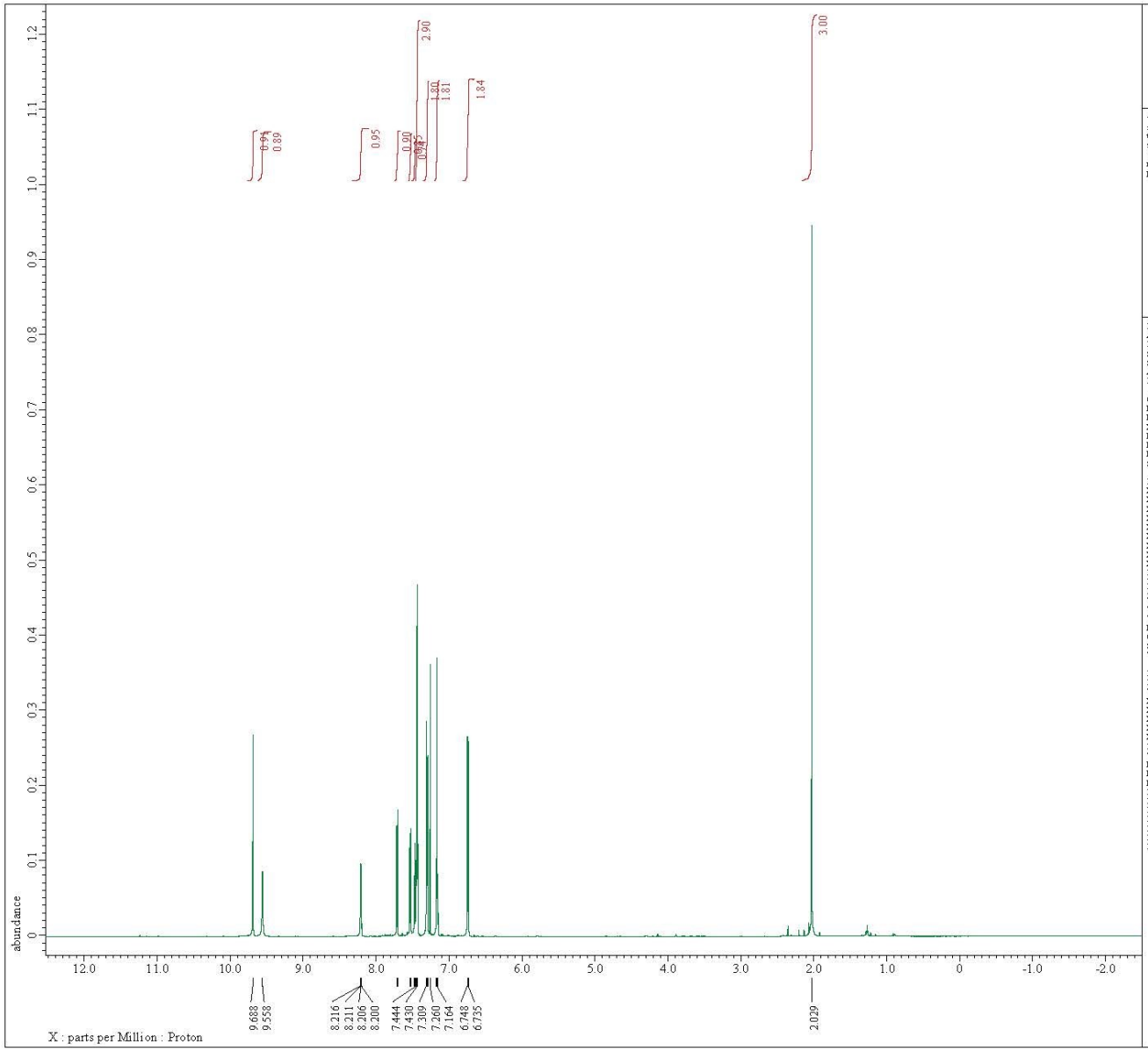




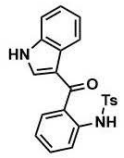
9ah

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

Filename	= Tk-6-085-3_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= Tk-6-085-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-APR-2024 15:23:20
Revision_Time	= 20-APR-2024 15:25:21
Comment	= single pulse decoupled gated NOE
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	= 36
Total_Scans	= 36
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21.3[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_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

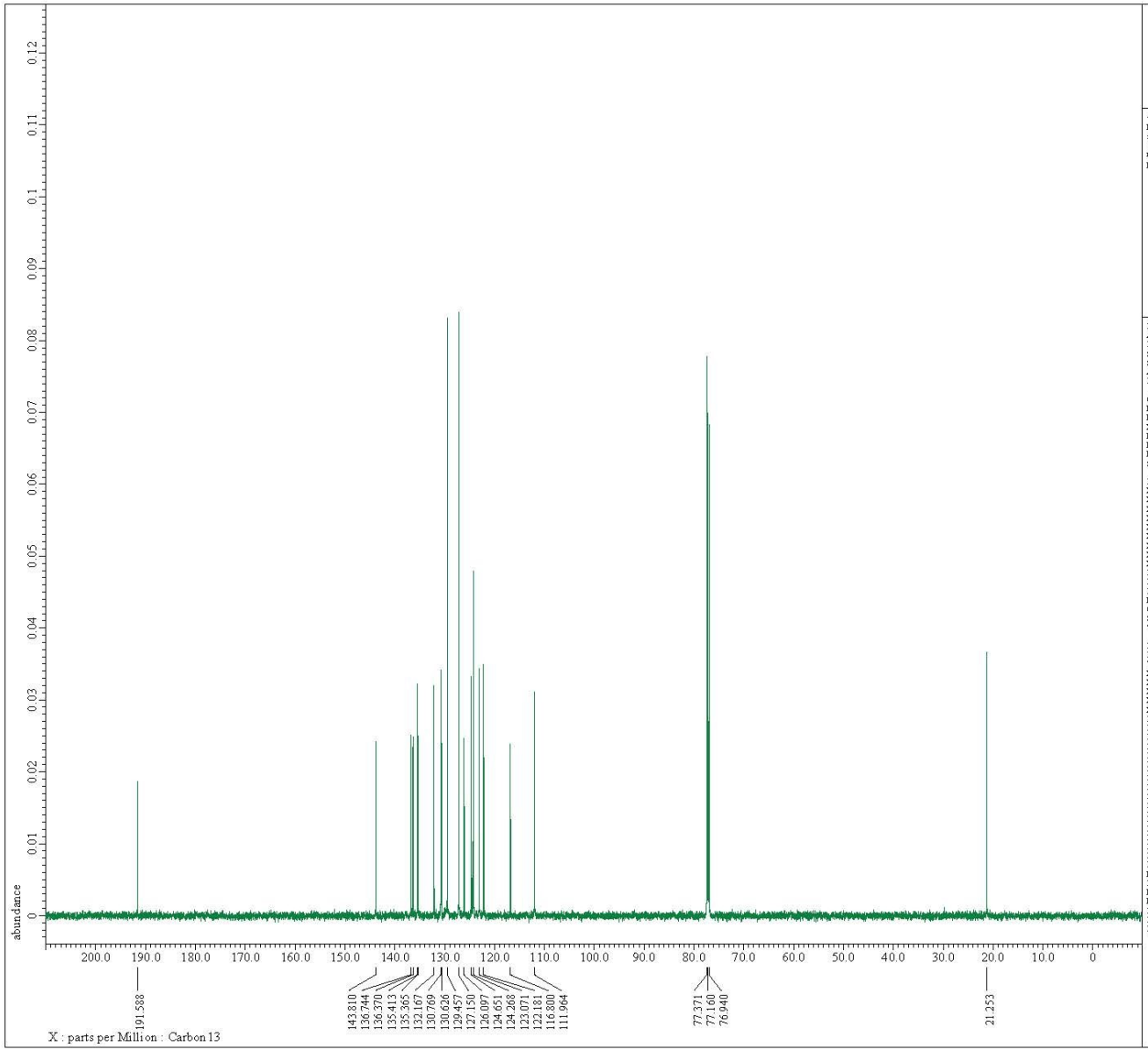


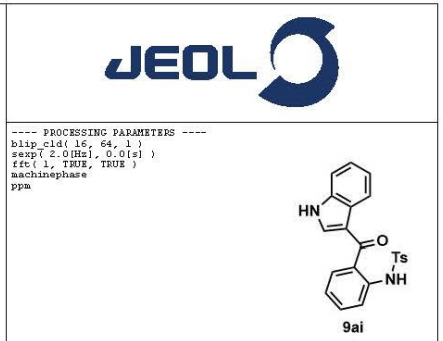
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm



9ai

Filename	= TK-6-084-2_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-6-084-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-APR-2024 14:51:57
Revision_Time	= 27-MAY-2024 22:09:59
Comment	= single_pulse
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	= 10[s]
Recvr_Gain	= 26
Temp_Get	= 20.5[dC]
X_90_Width	= 9.9[us]
X_Acq_Time	= 2.90455552[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 1000
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time	= 10[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 10[s]
Repetition_Time	= 12.90455552[s]

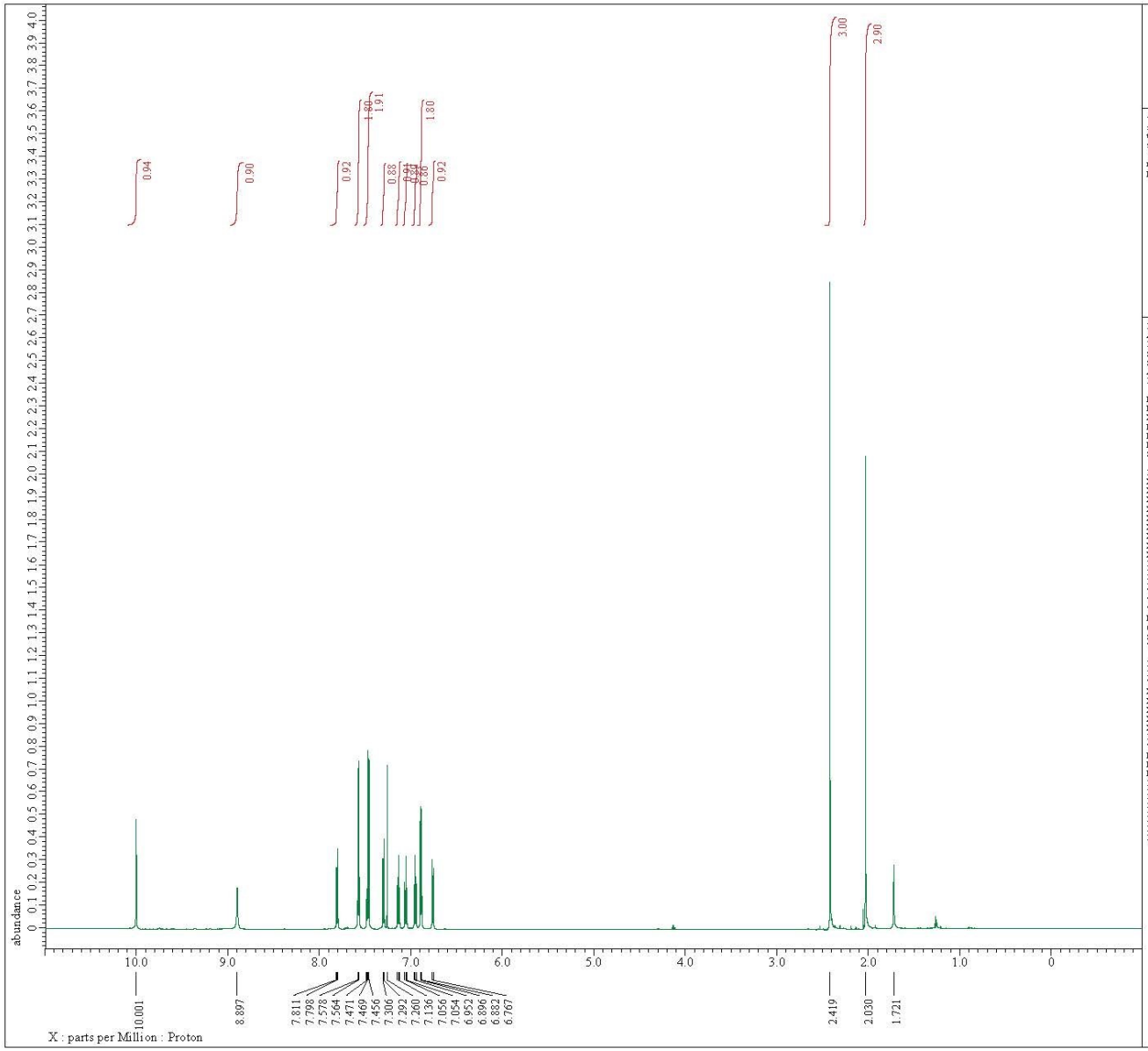


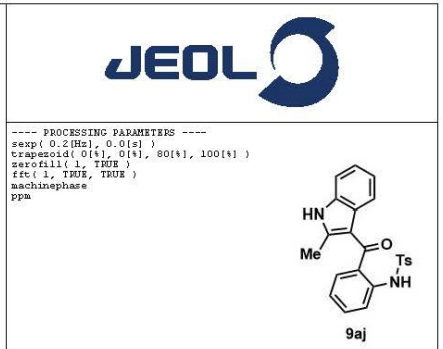


9ai

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

Filename	= TK-6-084-2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-084-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-APR-2024 14:55:22
Revision_Time	= 20-APR-2024 14:58:52
Comment	= single pulse decoupled gated NOE
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	= 80
Total_Scans	= 80
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[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_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

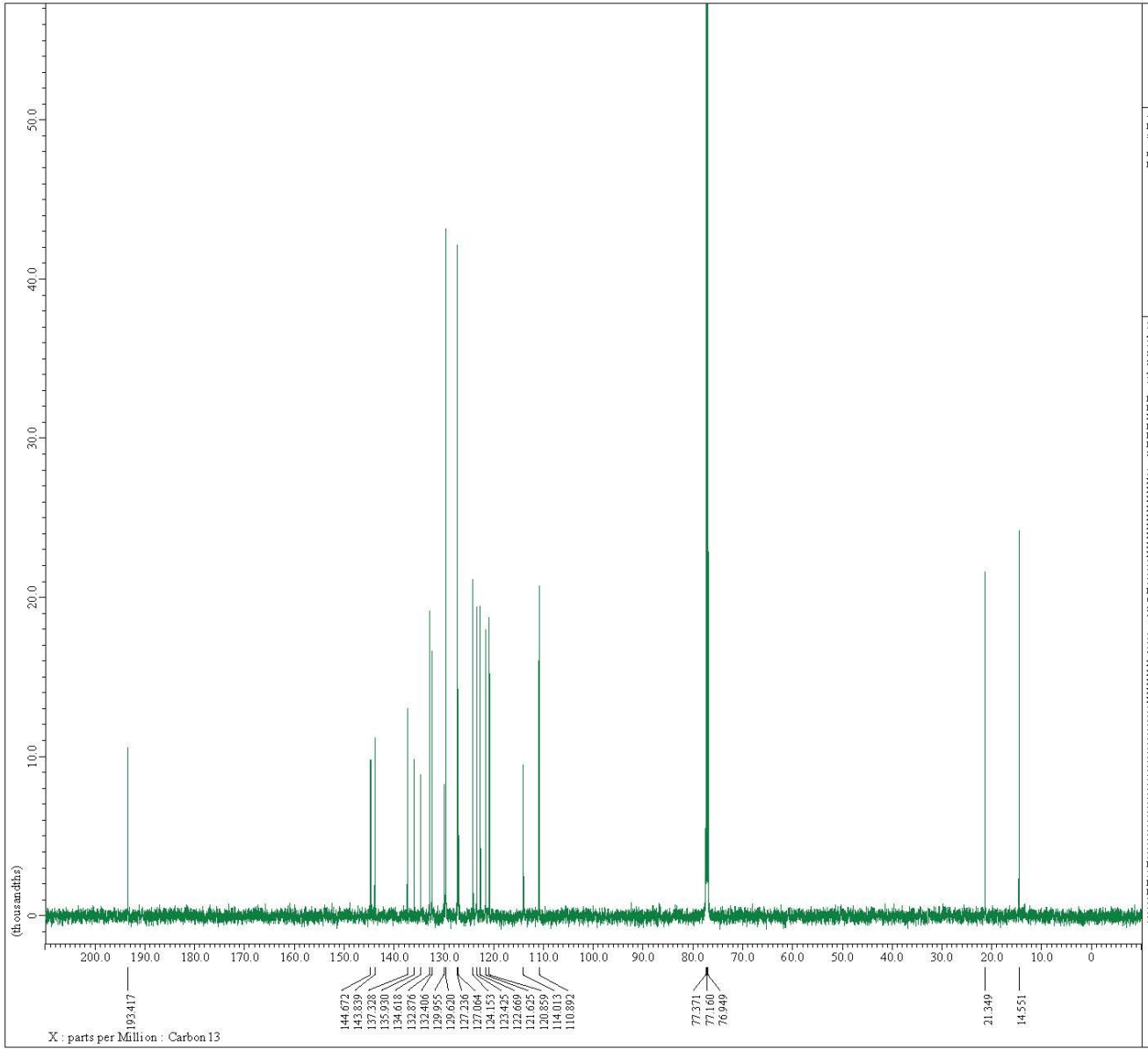


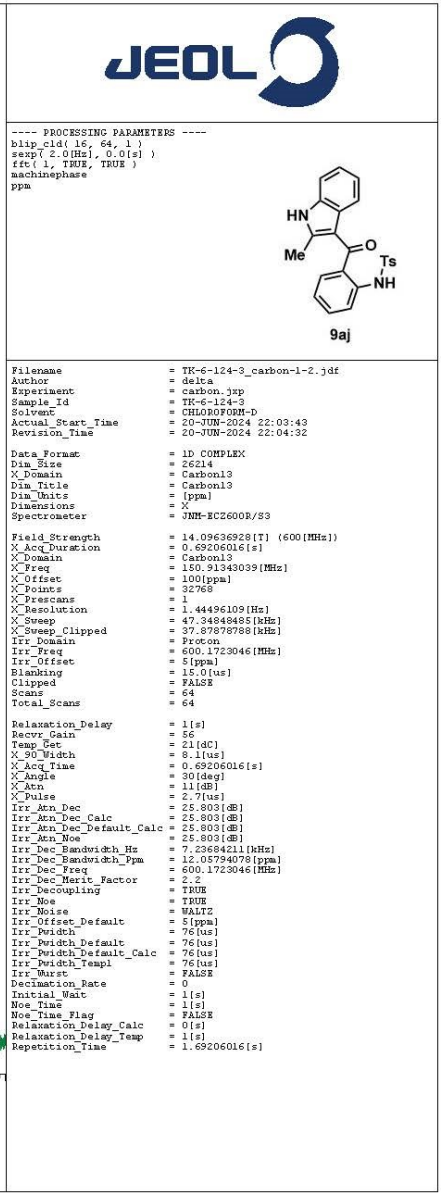


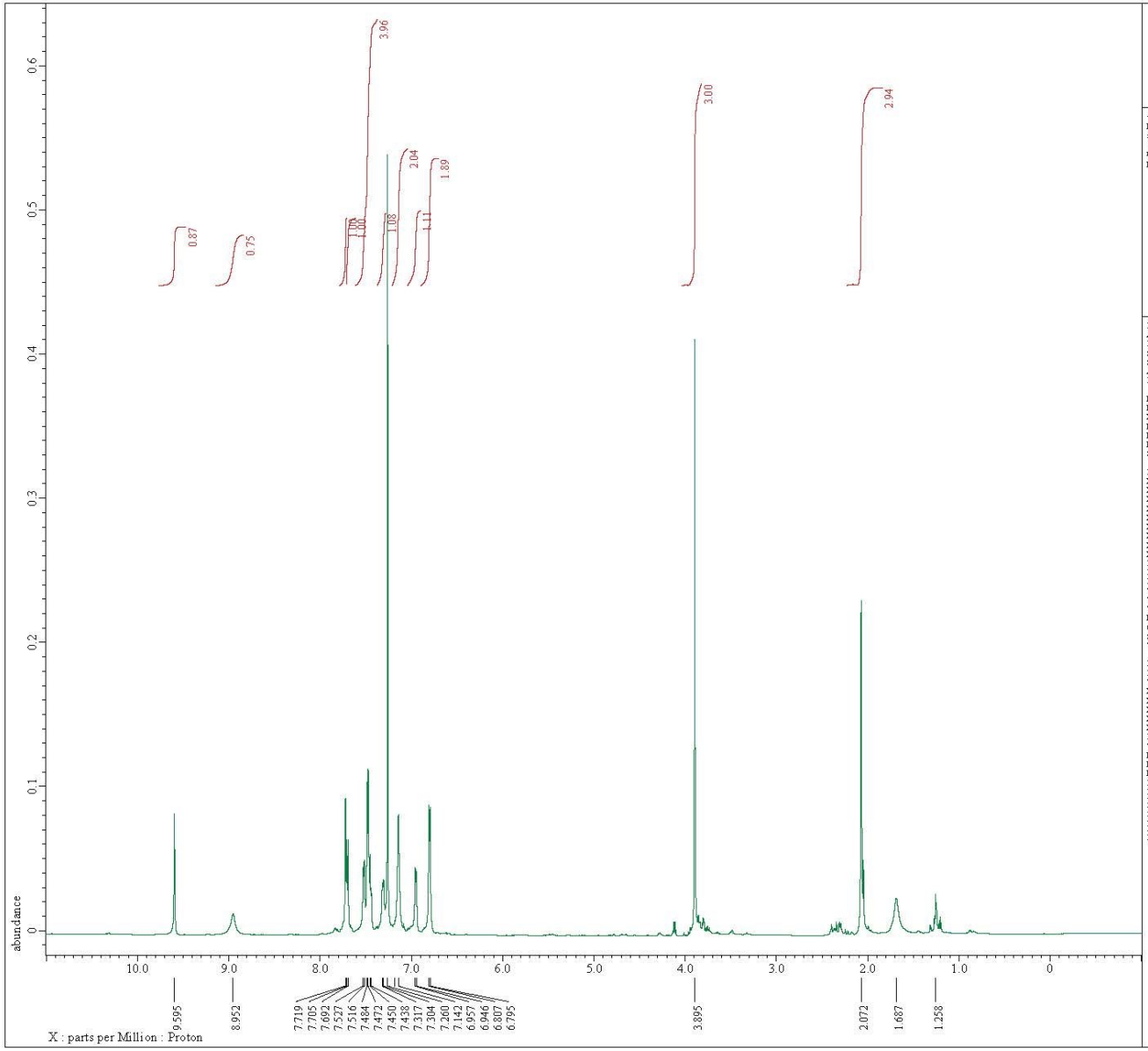
9aj

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

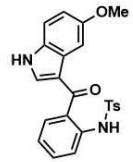
Filename	= TK-6-124-3_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-6-124-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JUN-2024 22:01:35
Revision_Time	= 24-JUN-2024 23:55:18
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= 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	= 36
Temp_Get	= 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	= {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.18365952[s]


(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
193.417
144.672
143.839
137.328
135.930
134.618
132.876
132.406
129.955
129.620
127.236
127.064
124.153
123.425
122.669
121.625
120.859
114.013
110.892
77.371
77.160
76.949
21.349
14.551
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
HN
Me
O
Ts
NH
9aj
Filename = TK-6-124-3_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-124-3
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-JUN-2024 22:03:43
Revision_Time = 20-JUN-2024 22:04:32
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 = 64
Total_Scans = 64
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 21[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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]



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



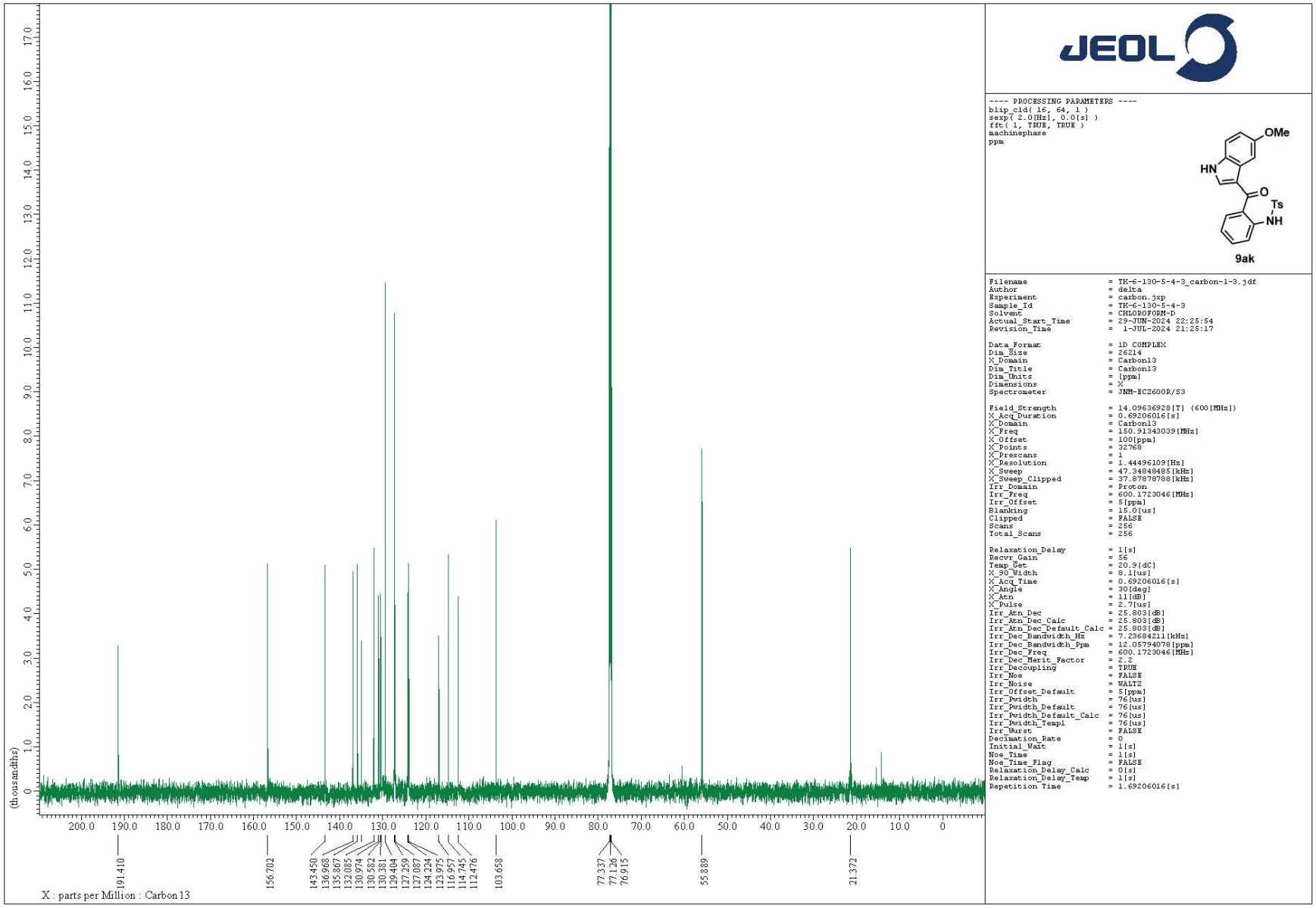
9ak

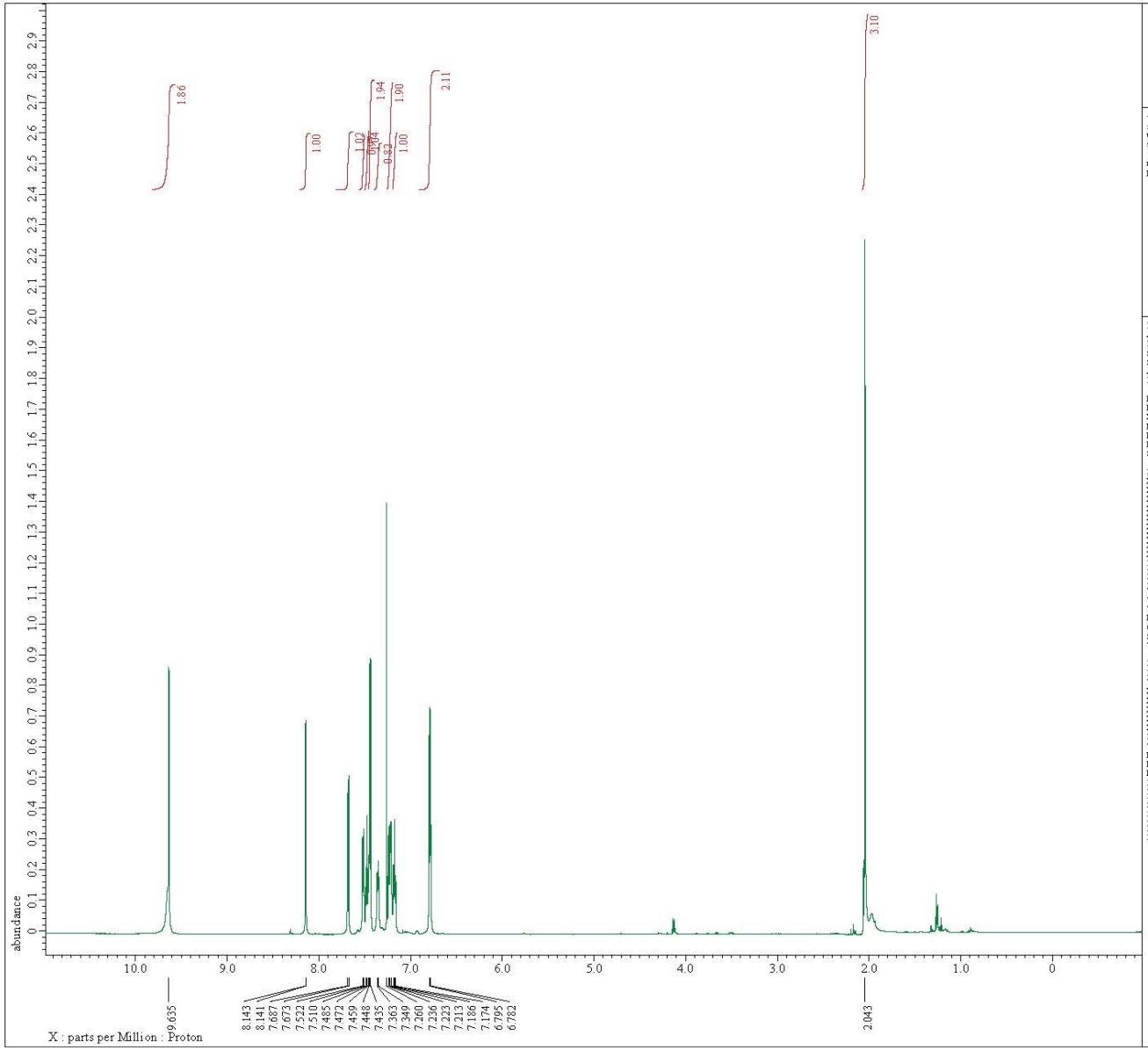
Filename = TK-6-130-5-4-3_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-130-5-4-3
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JUN-2024 22:23:09
Revision_Time = 1-JUL-2024 23:41:44

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

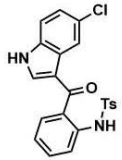
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 15.0060024[kHz]
X_Sweep_Clipped = 12.00480192[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 32
Total_Scans = 32

Relaxation_Delay = 2[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 = 4.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18365952[s]


(thousandths)
X : parts per Million : Carbon13
191.410
156.702
143.450
136.968
135.867
132.085
130.974
130.582
130.381
129.404
127.259
127.087
124.224
123.975
116.957
114.745
112.476
103.658
77.337
77.126
76.915
55.889
21.372
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
OMe
HN
O
Ts
NH
9ak
Filename = TK-6-130-5-4-3_carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-130-5-4-3
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JUN-2024 22:25:54
Revision_Time = 1-JUL-2024 21:25:17
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 = 256
Total_Scans = 256
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Set = 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_Default_Calc = 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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = FALSE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]



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



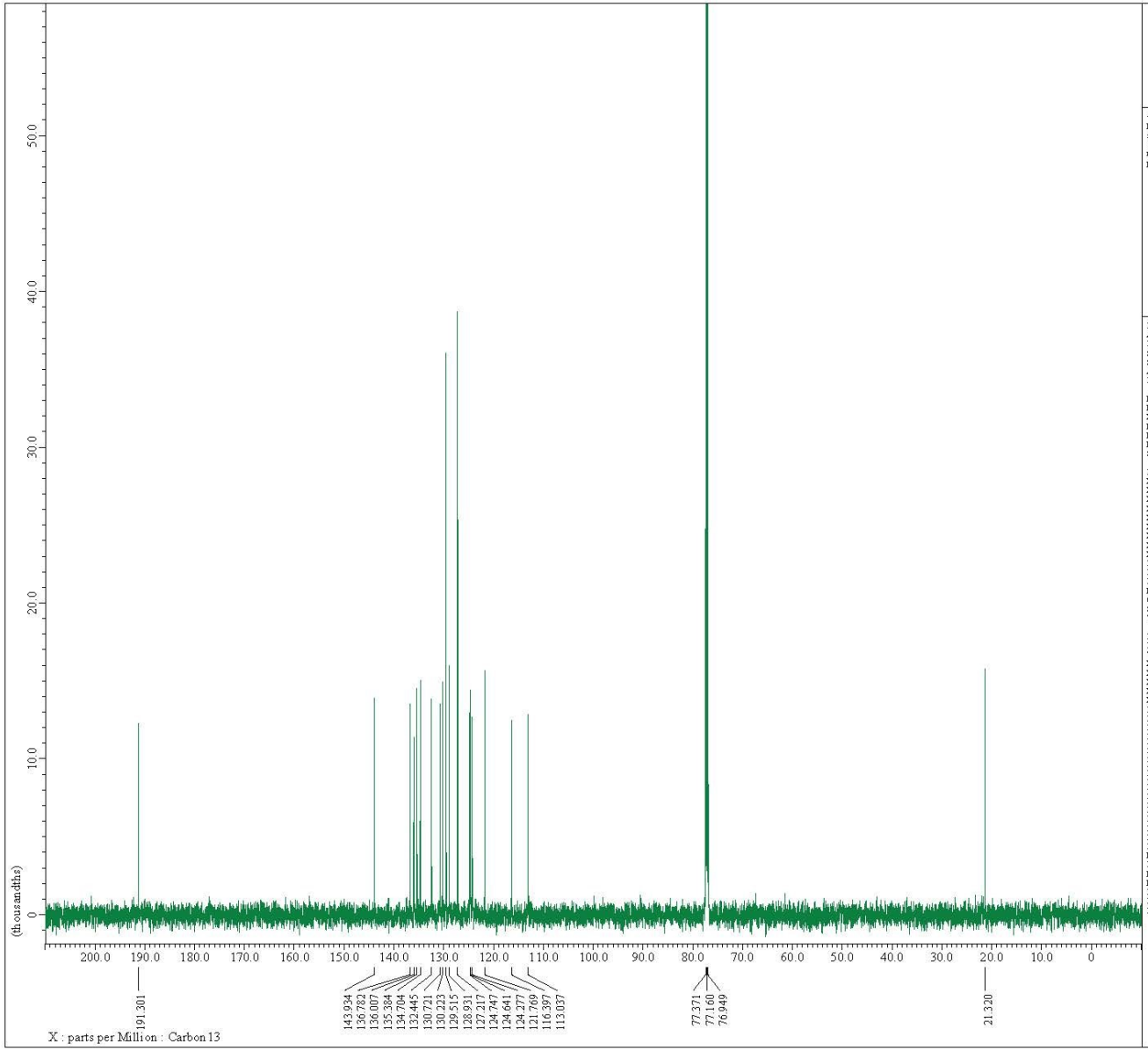
9al

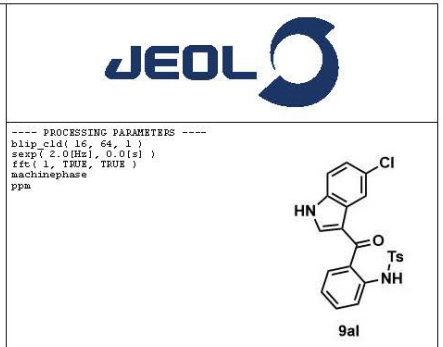
Filename = TK-6-125-1_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-125-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-JUN-2024 22:39:20
Revision_Time = 28-JUN-2024 16:33:44

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 = 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 = 4.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18365952[s]

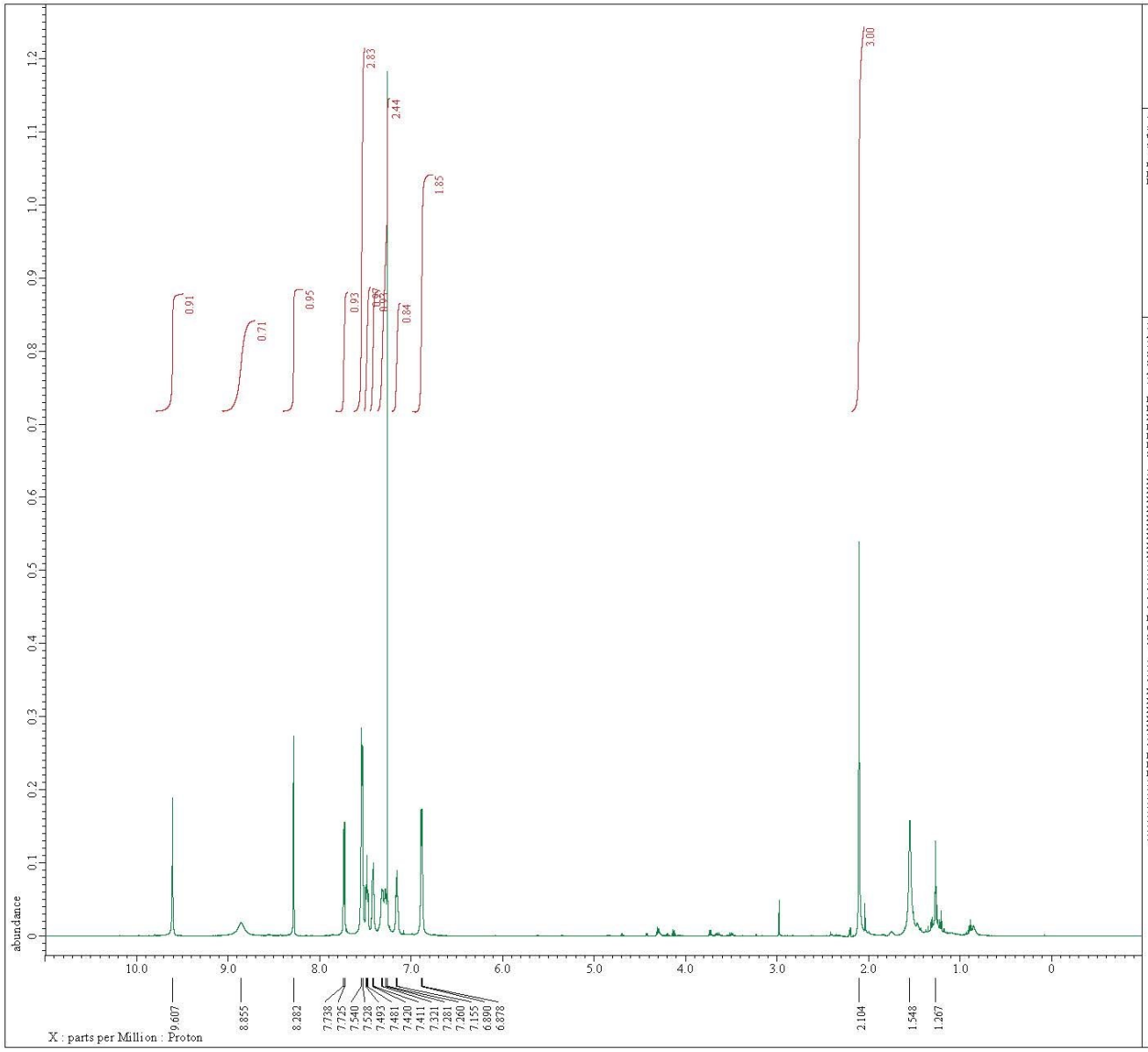


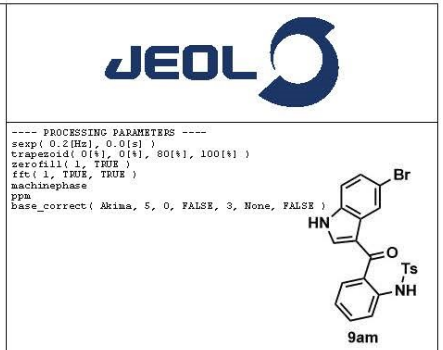



```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```


9al

Filename	= TK-6-125-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-125-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2024 22:41:24
Revision_Time	= 25-JUN-2024 22:39:39
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	= 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	= 32
Total_Scans	= 32
Relaxation_Delay	= 1[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Declination_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

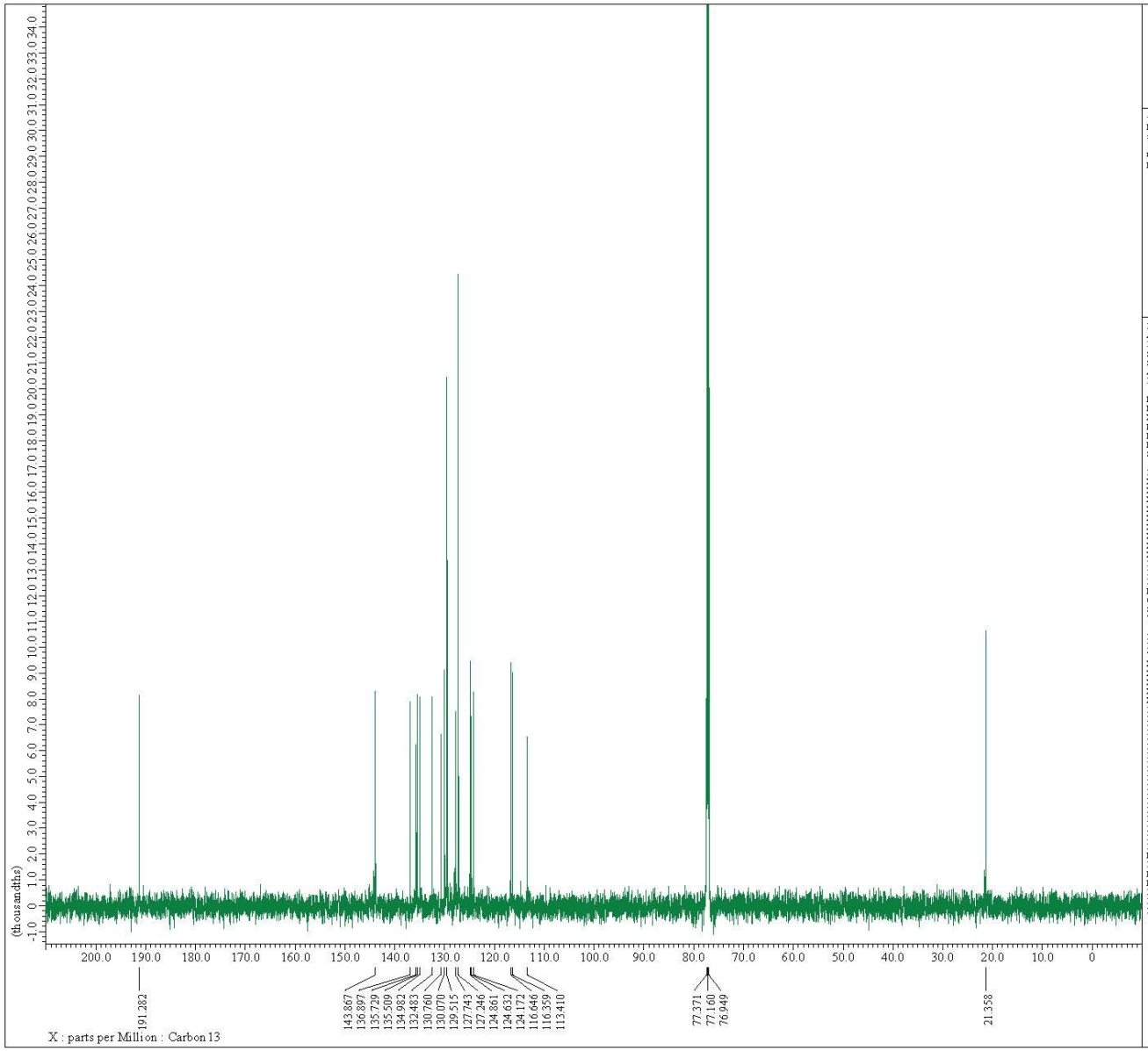


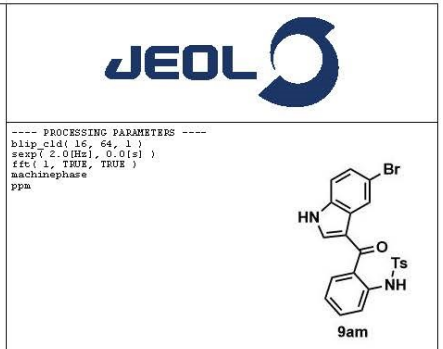



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FALSE )
```


9am

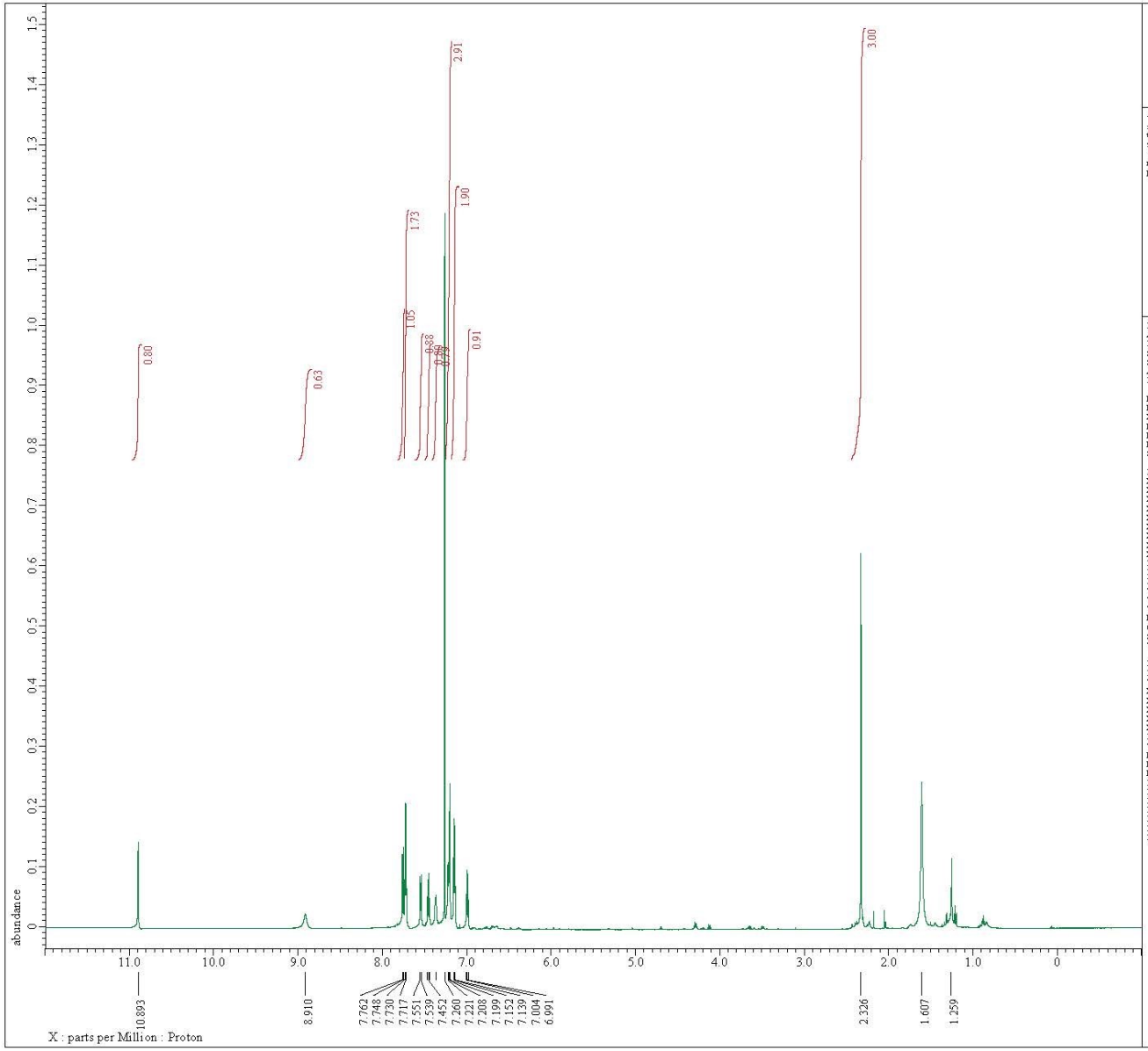
```
Filename                = TK-6-137-5-2_proton-4-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-137-5-2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  1-JUL-2024 20:12:29
Revision_Time           =  1-JUL-2024 20:23:35

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[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              = 46
Temp_Set                = 45[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
RelaxationDelay_Calc    = 0[s]
RelaxationDelay_Temp    = 2[s]
Repetition_Time         = 4.18365952[s]
```



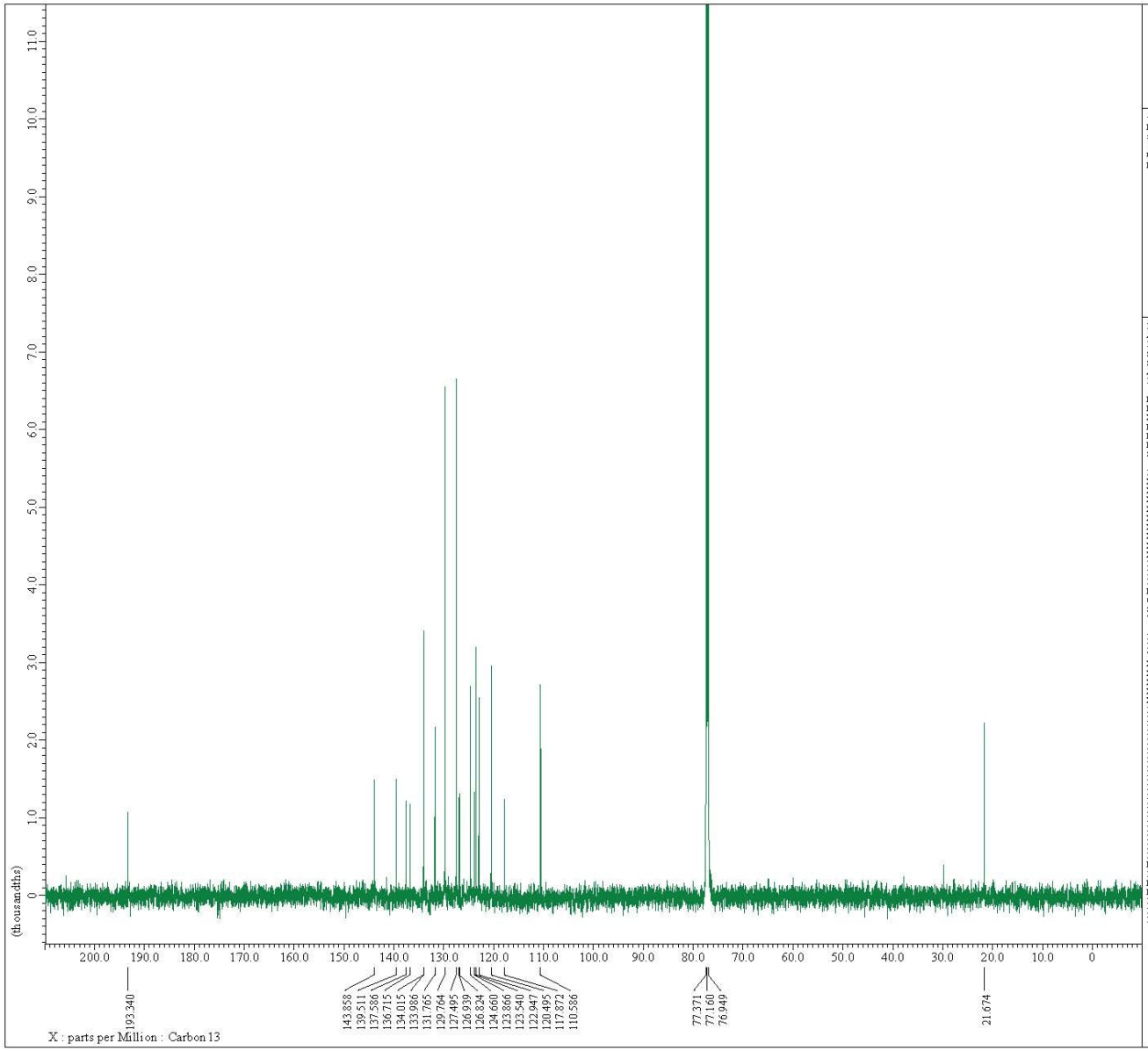


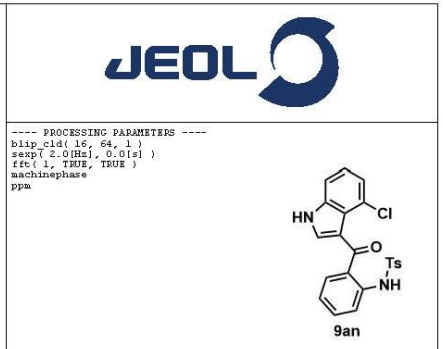

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= TK-6-137-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-137-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2024 22:56:24
Revision_Time	= 25-JUN-2024 22:55:42
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	= 64
Total_Scans	= 64
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 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_Default_Calc	= 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_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]


abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.893
8.910
7.762
7.748
7.730
7.717
7.551
7.539
7.452
7.260
7.221
7.208
7.199
7.152
7.139
7.004
6.991
2.326
1.607
1.259
X : parts per Million : Proton


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
HN
Cl
O
Ts
NH
9an
Filename = TK-6-128-5_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-128-5
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-JUN-2024 21:33:24
Revision_Time = 25-JUN-2024 12:05:37
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 = 46
Temp_Set = 20.7[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 = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18365952[s]

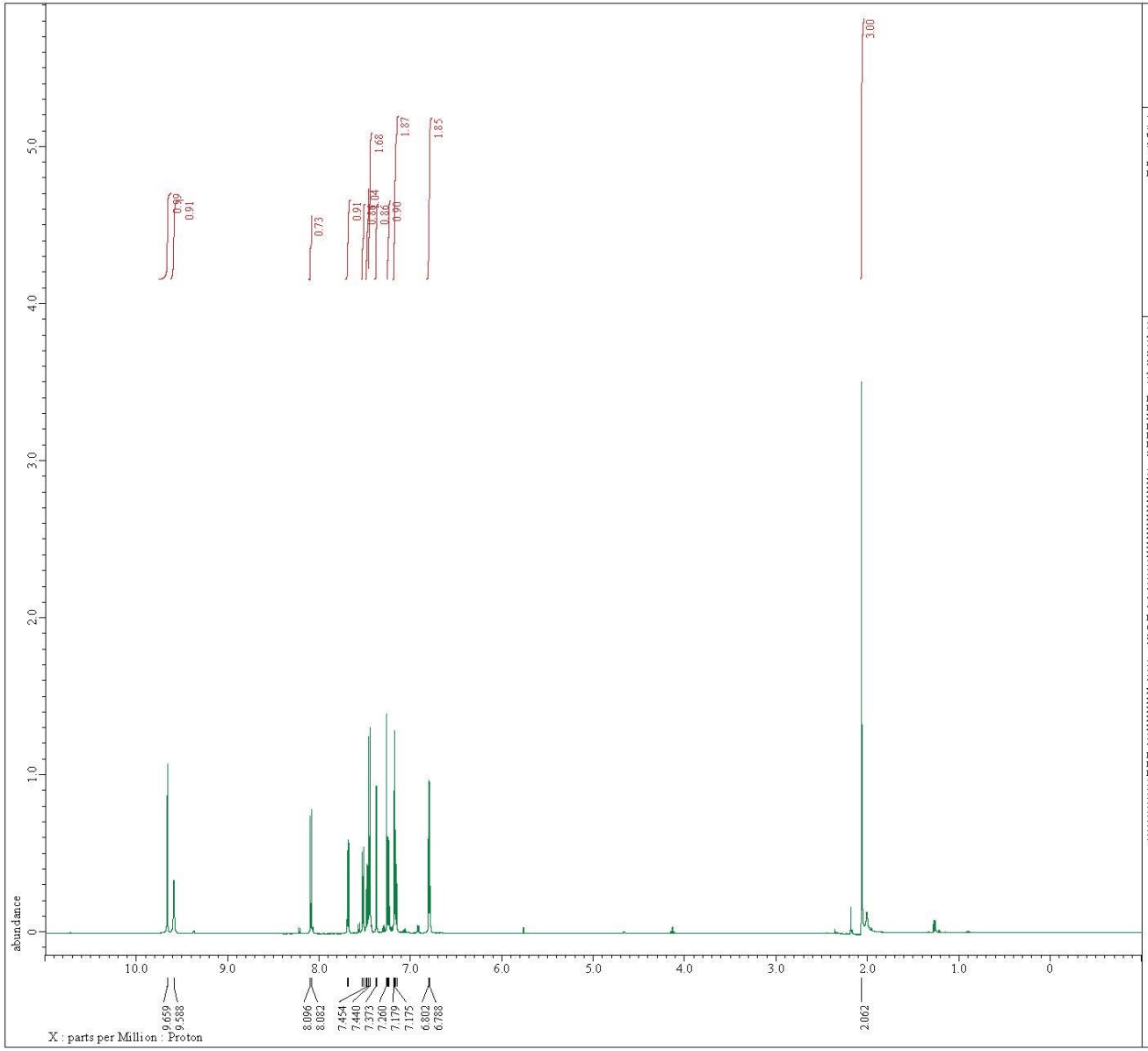




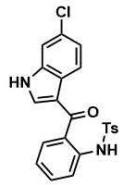
9an

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

Filename	= TK-6-128-5_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-128-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JUN-2024 21:35:33
Revision_Time	= 20-JUN-2024 21:58:37
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	= 512
Total_Scans	= 512
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 21.1[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	= 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

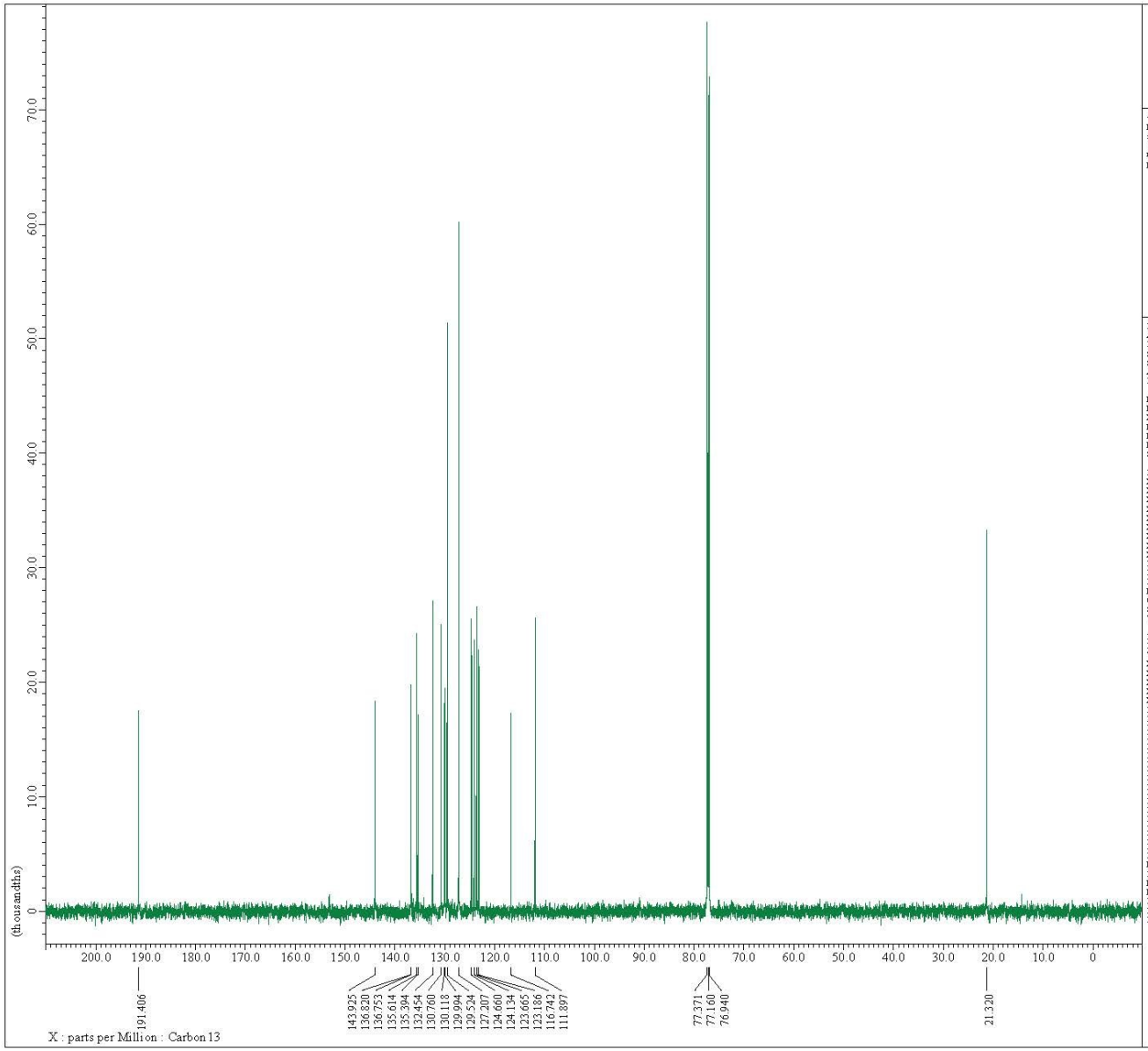


---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm

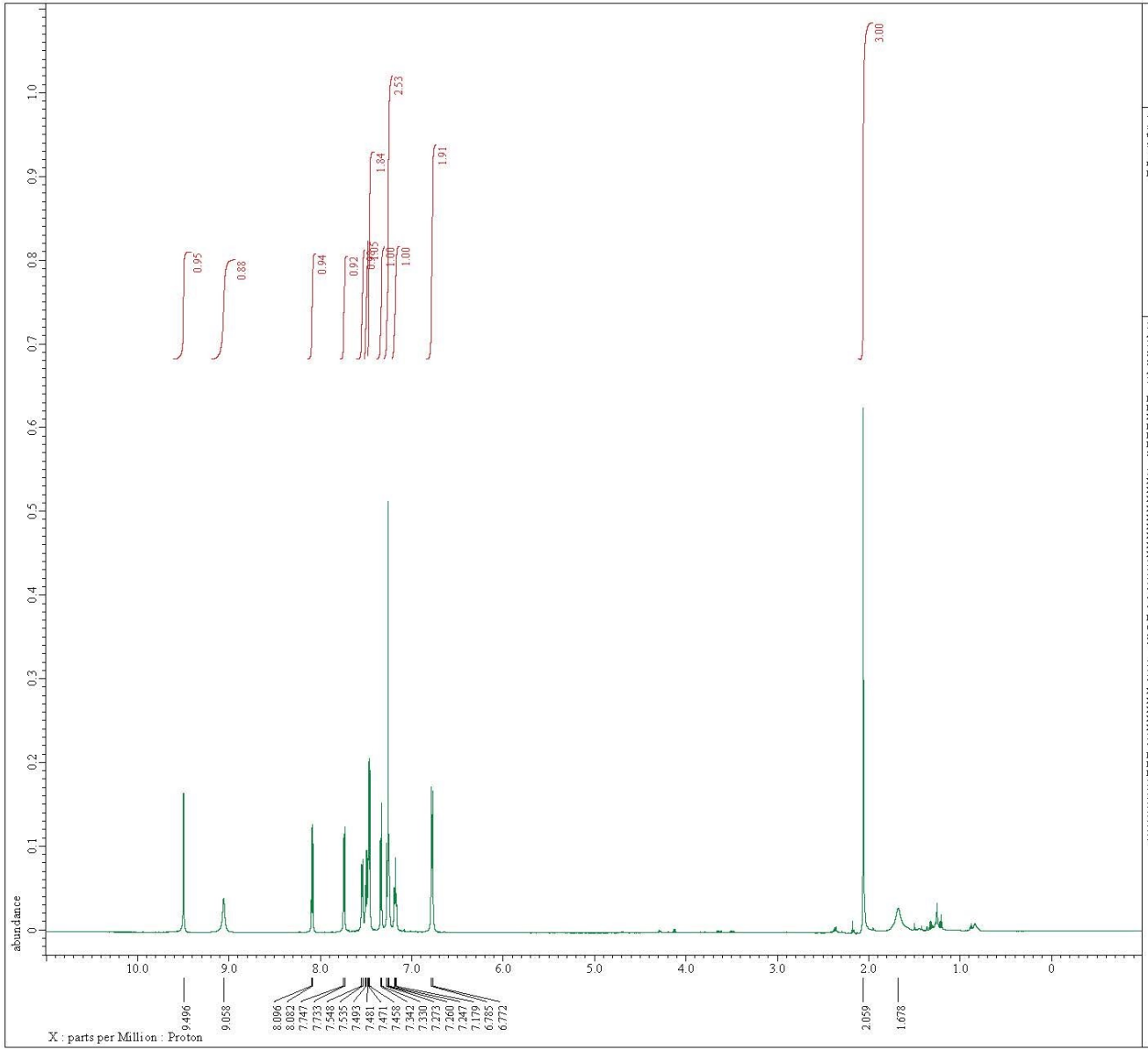


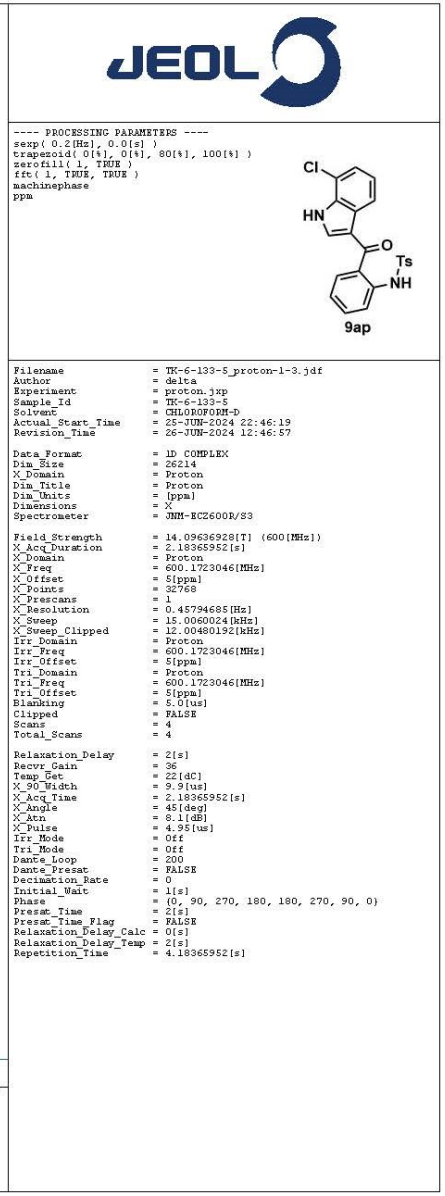
9ao

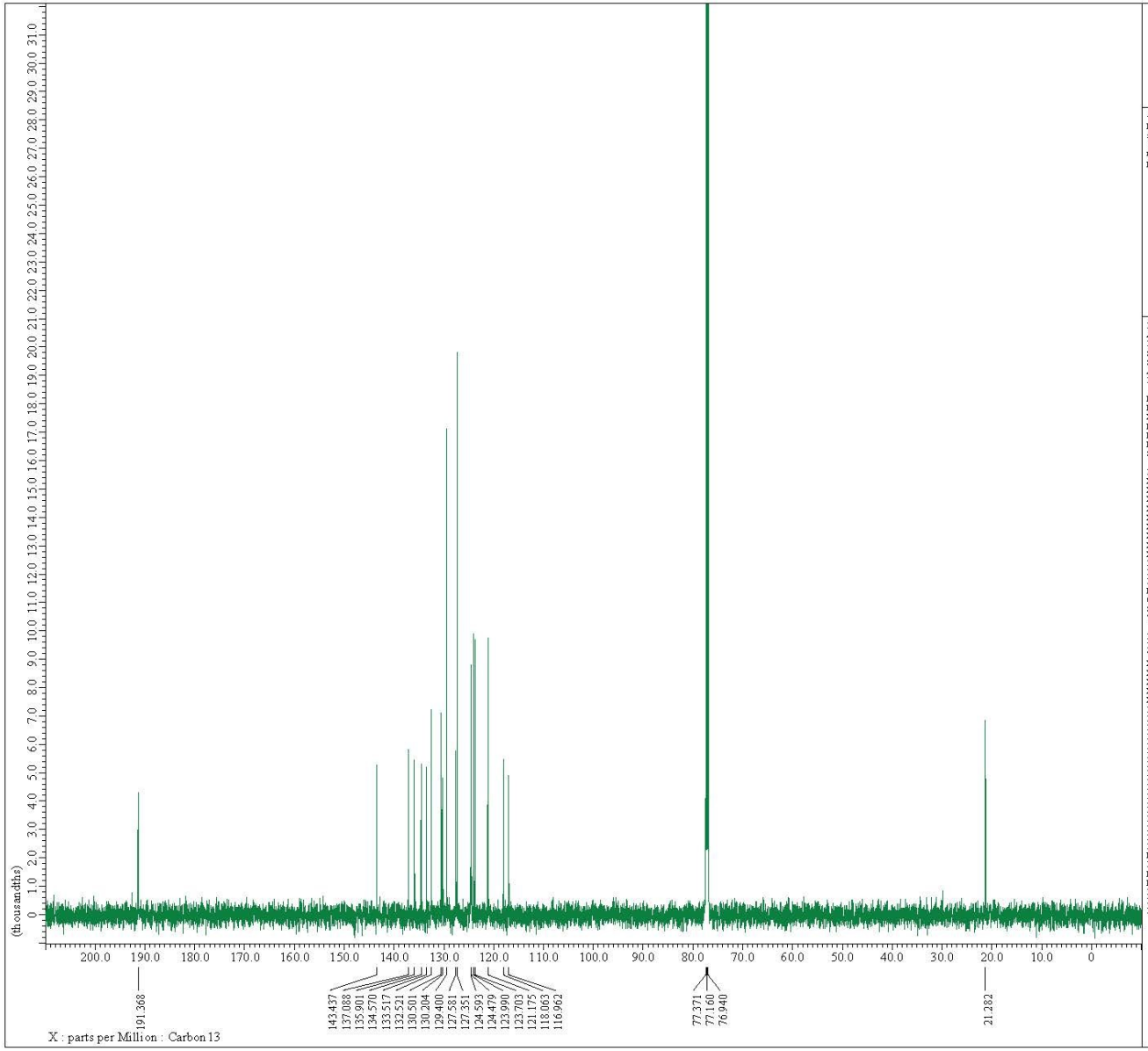
Filename	= TK-6-221-1_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-6-221-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-JUN-2024 20:40:54
Revision_Time	= 17-JUN-2024 15:28:15
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= 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	= 36
Temp_Set	= 20.8[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	= (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.18365952[s]

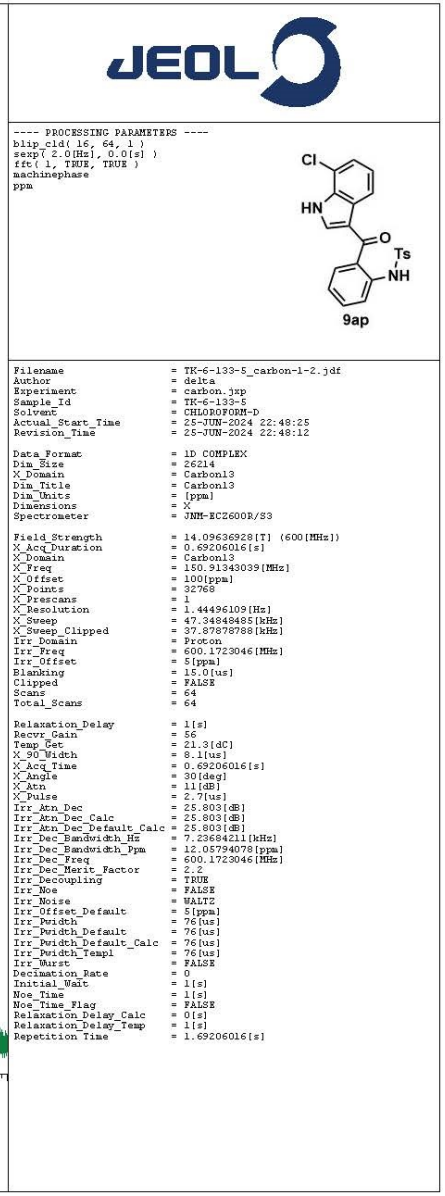

(thousandths)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
191.406
143.925
136.820
136.753
135.614
135.394
132.454
130.760
130.118
129.994
129.524
127.207
124.660
124.134
123.665
123.186
116.742
111.897
77.371
77.160
76.940
21.320
X : parts per Million : Carbon13


---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
Cl
HN
O
Ts
NH
9ao
Filename = TK-6-221-1_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-221-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-JUN-2024 20:43:03
Revision_Time = 16-JUN-2024 20:42:07
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 = 45
Total_Scans = 45
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Set = 21.1[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 = 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]


abundance
X : parts per Million : Proton
9.496
9.058
8.096
8.082
7.747
7.733
7.548
7.535
7.493
7.481
7.471
7.458
7.342
7.330
7.273
7.260
7.247
7.179
6.785
6.772
2.059
1.678
0.95
0.88
0.94
0.92
0.80
0.80
1.00
1.00
1.84
2.53
1.91
3.00


---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Cl
HN
O
Ts
NH
9ap
Filename = TK-6-133-5_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-133-5
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-JUN-2024 22:46:19
Revision_Time = 26-JUN-2024 12:46:57
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 = 36
Temp_Set = 22[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 = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18365952[s]

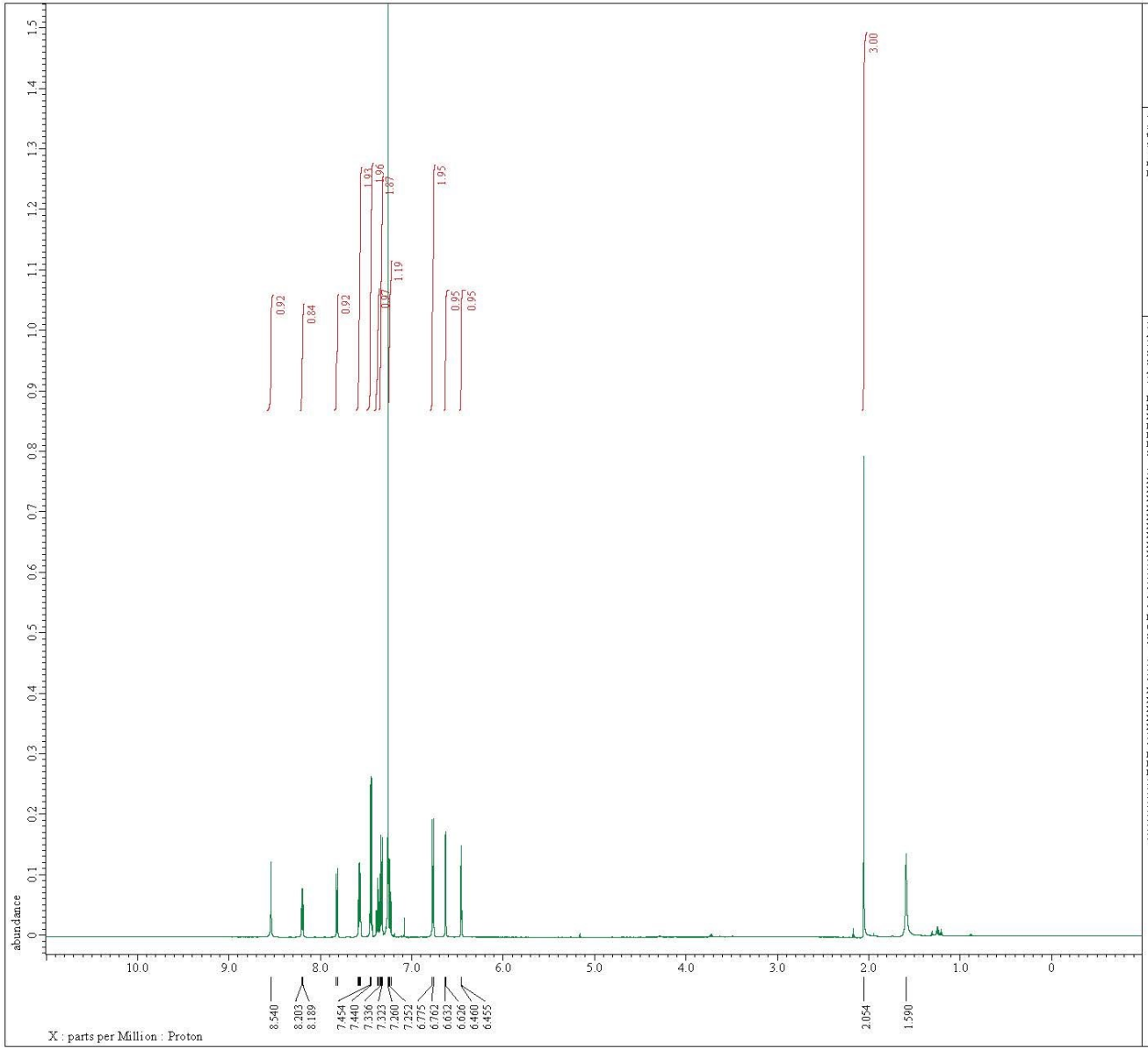




```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```


9ap

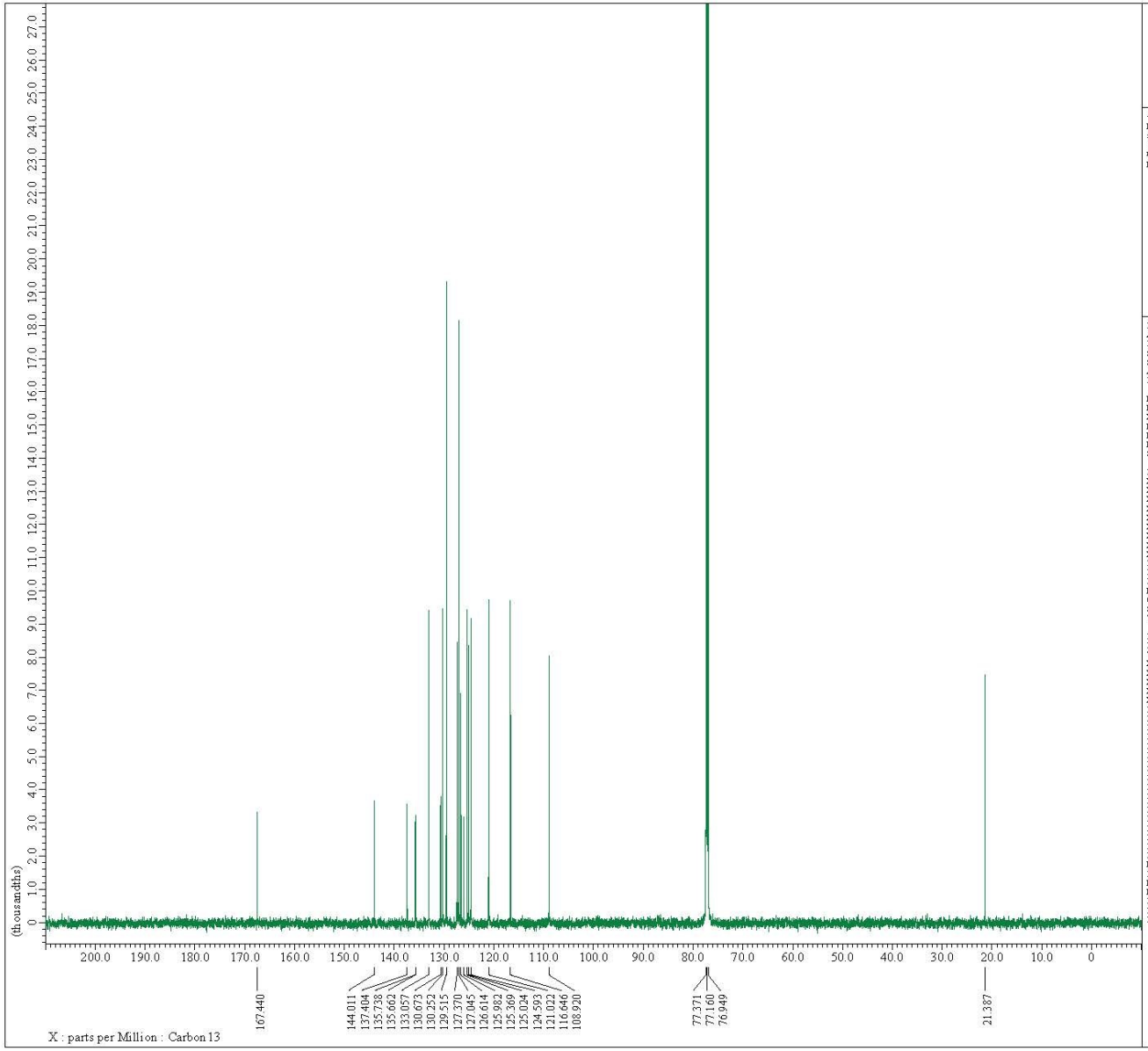
Filename	= TK-6-133-5_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-133-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2024 22:48:25
Revision_Time	= 25-JUN-2024 22:48:12
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 64
Total_Scans	= 64
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21.3[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Declination_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



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

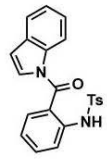

9aq

```
Filename                = TK-6-126-5-4_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-126-5-4
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 23-JUN-2024 12:23:57
Revision_Time           = 24-JUN-2024 23:33:55

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        = 2[s]
Recvr_Gain              = 36
Temp_Set                = 21.4[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```



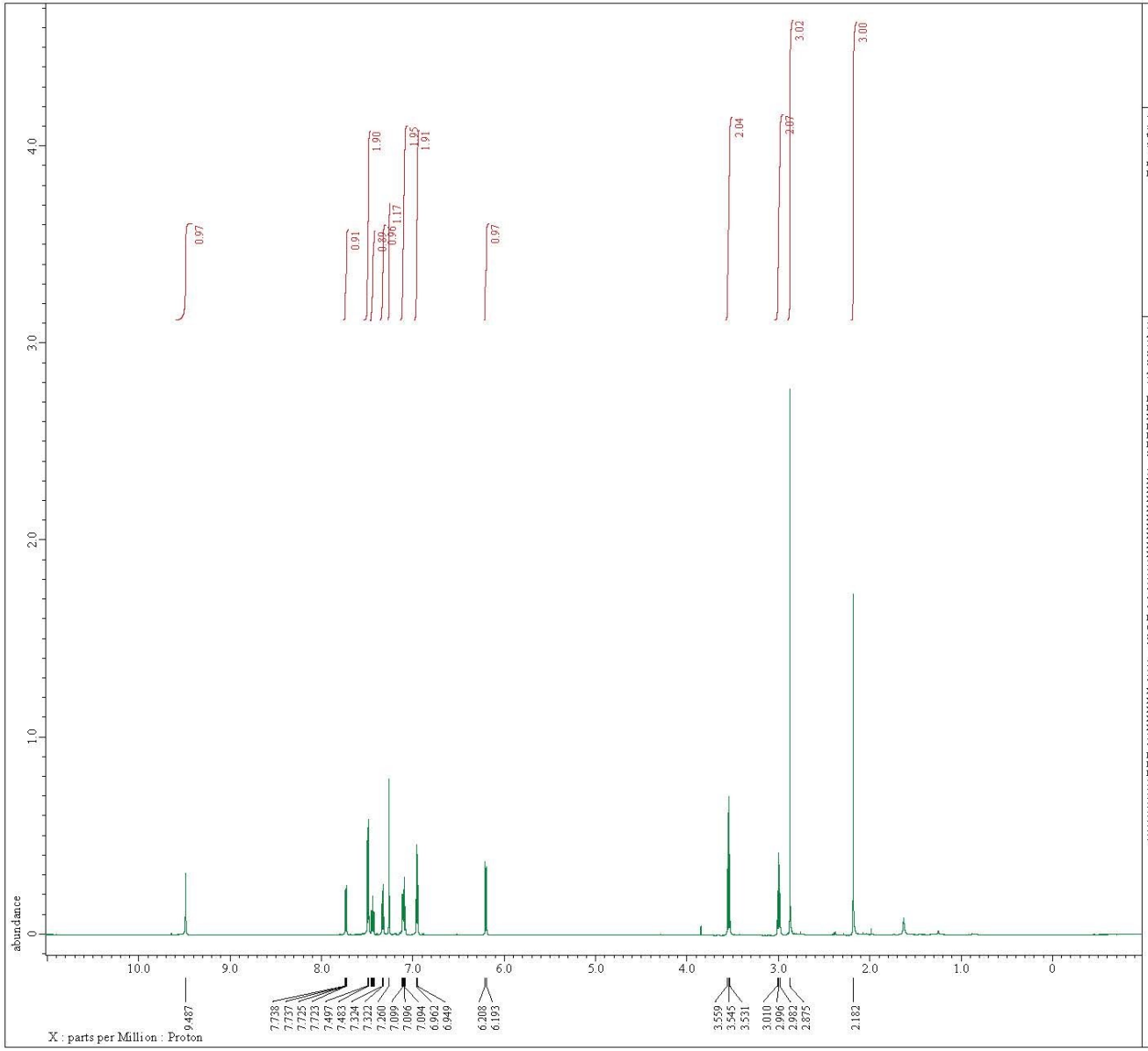
JEOL

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

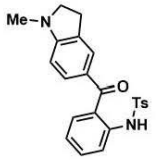


9aq

Filename	= TK-6-126-5-4_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-126-5-4
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JUN-2024 12:26:02
Revision_Time	= 23-JUN-2024 13:26:05
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	= 512
Total_Scans	= 512
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21.6[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_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

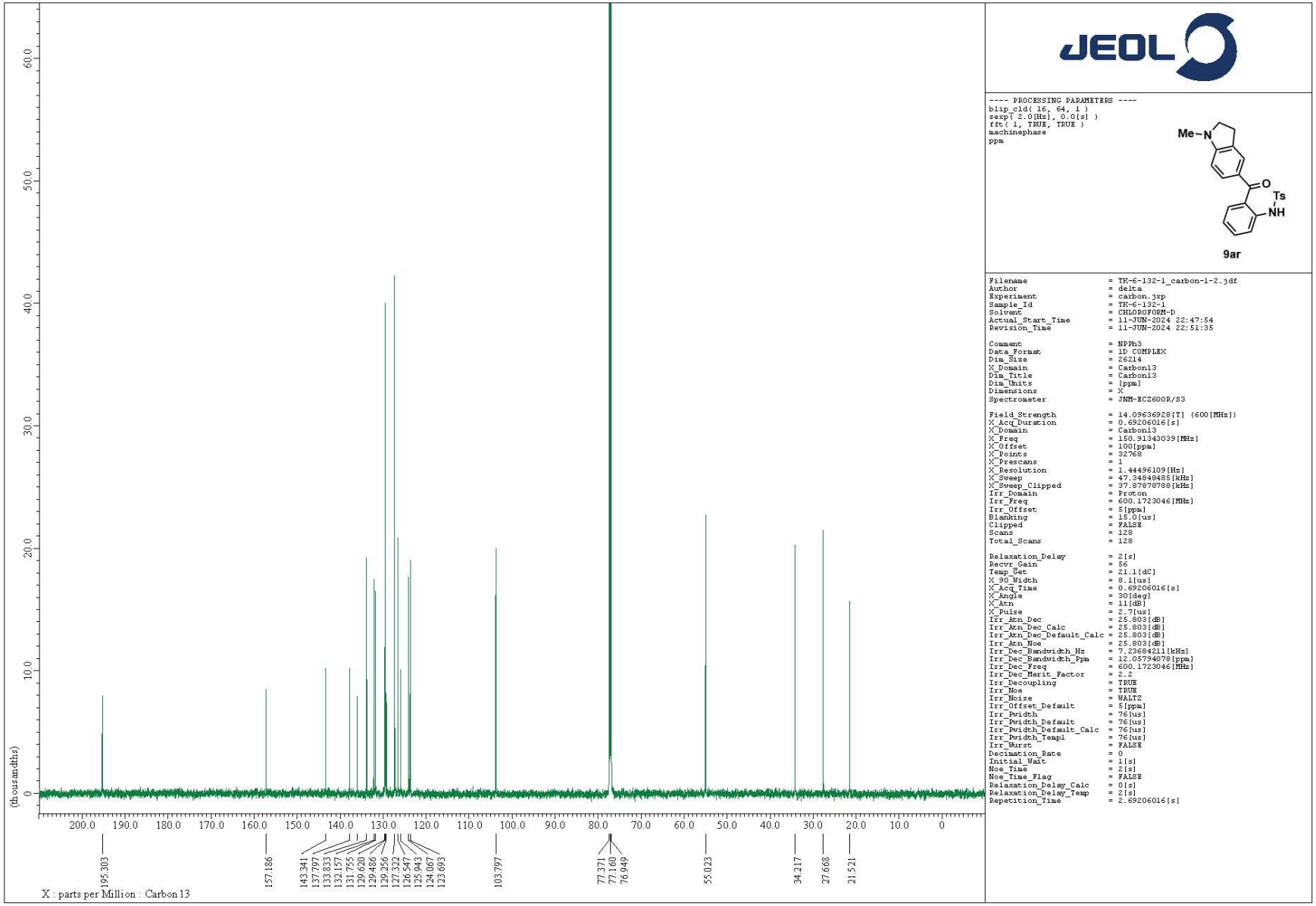



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```



9ar

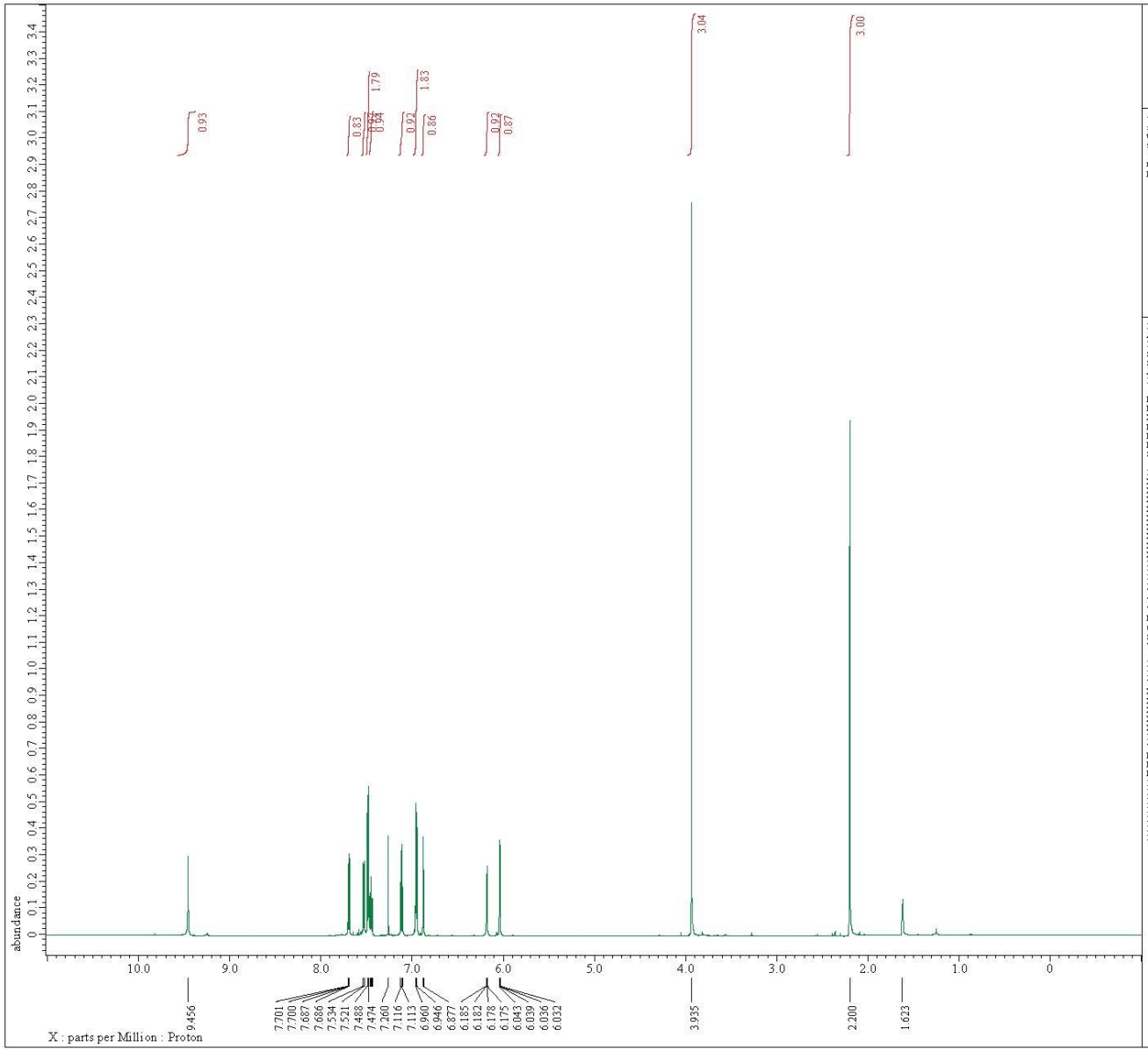
```
Filename                = TK-6-132-1_proton-2-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-132-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 11-JUN-2024 22:28:36
Revision_Time           =  3-JUL-2024 13:17:37

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              = 36
Temp_Set                = 21.8[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```



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

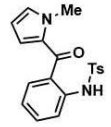
9ar

Filename	= TK-6-132-1_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-132-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-JUN-2024 22:47:54
Revision_Time	= 11-JUN-2024 22:51:35
Comment	= NPPh3
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	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 21.1[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	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 2.69206016[s]



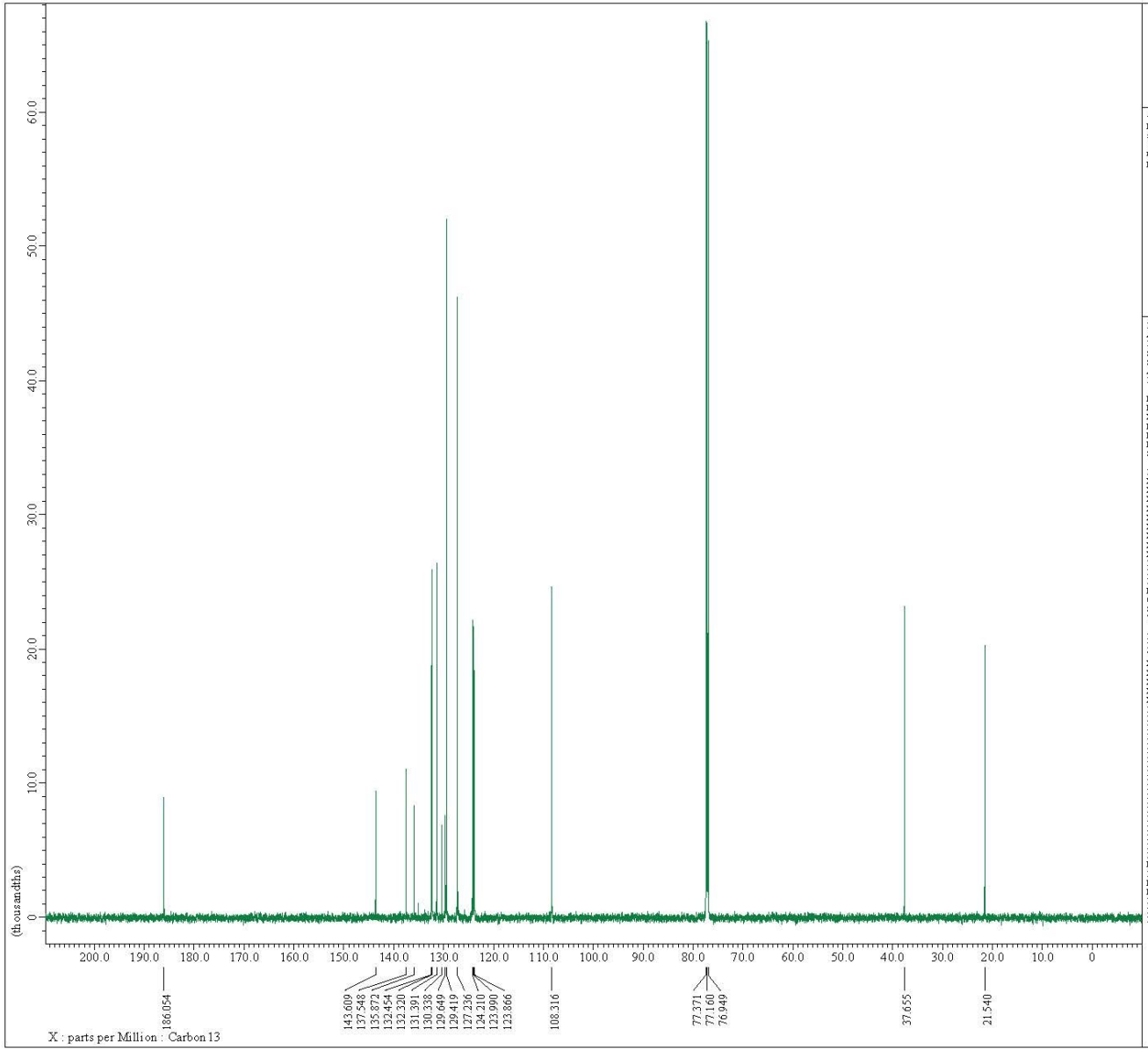
JEOL

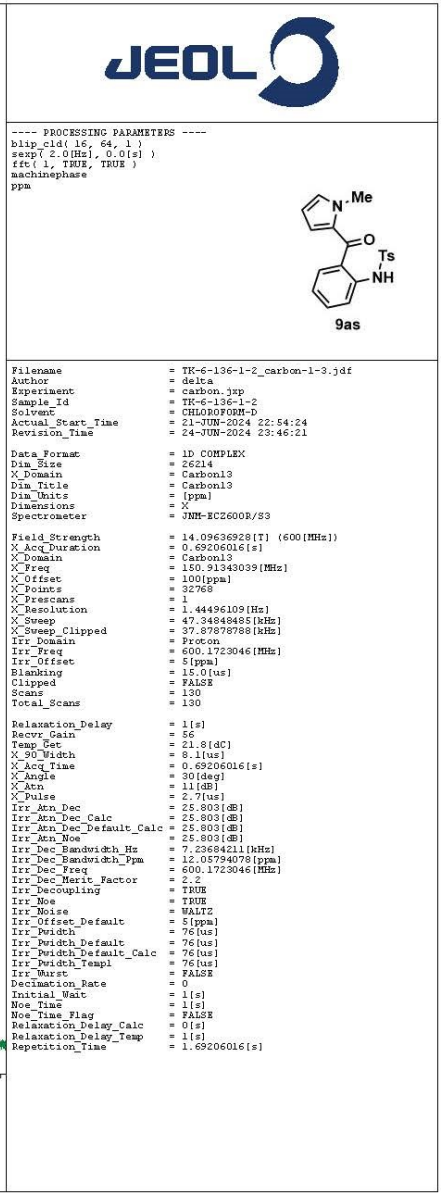
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

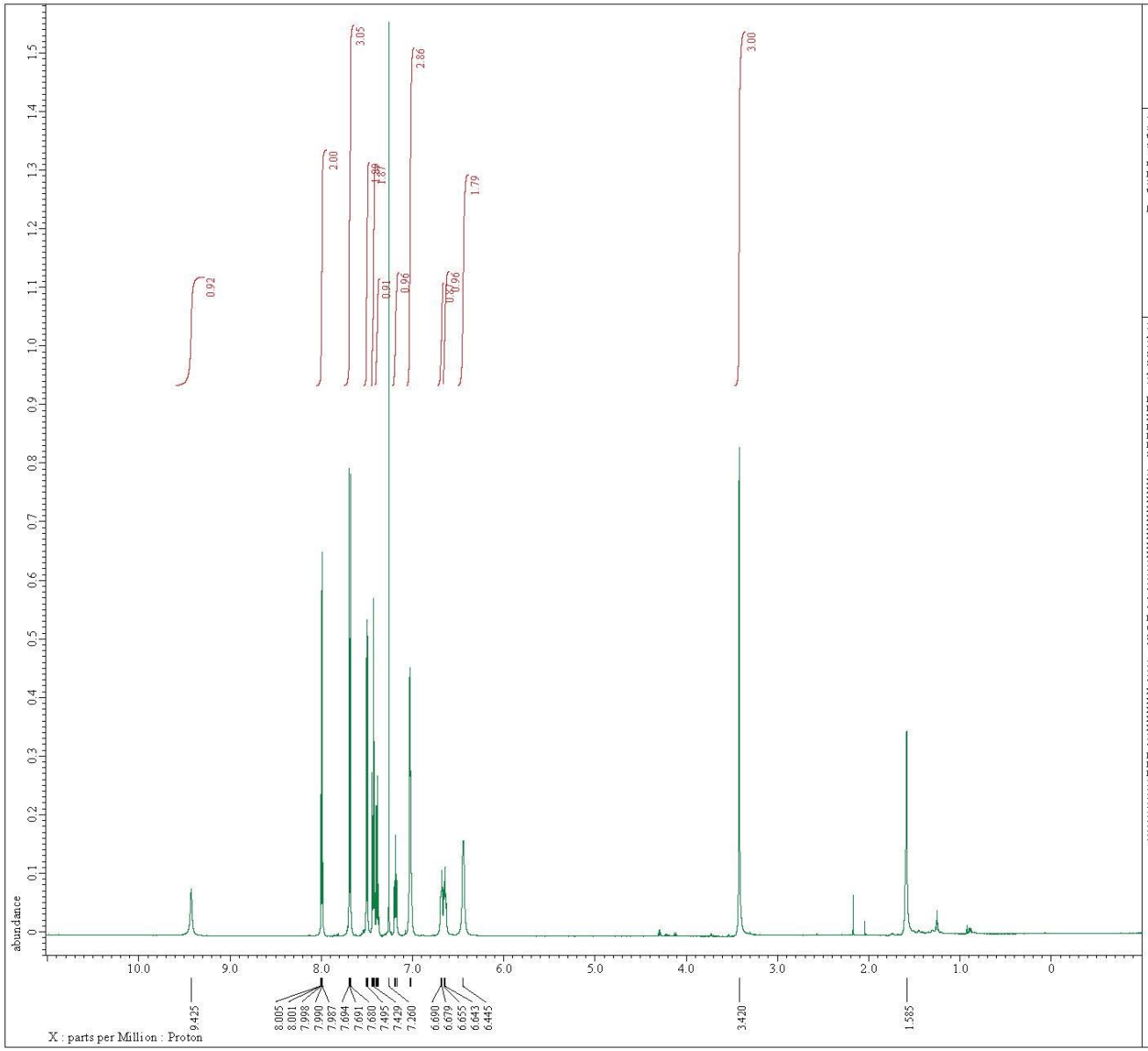


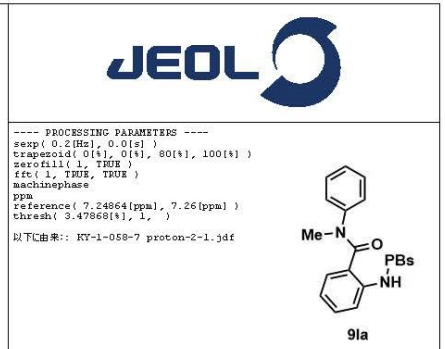
9as

```
Filename                = TK-6-136-1-2_proton-1-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-136-1-2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 21-JUN-2024 22:51:58
Revision_Time           = 24-JUN-2024 23:44:19

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                   = 8
Total_Scans             = 8

Relaxation_Delay        = 2[s]
Recvr_Gain              = 36
Temp_Get                = 21.9[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
RelaxationDelay_Calc    = 0[s]
RelaxationDelay_Temp    = 2[s]
Repetition_Time         = 4.18365952[s]
```


(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
186.054
143.609
137.548
135.872
132.454
132.320
131.391
130.338
129.649
129.419
127.236
124.210
123.990
123.866
108.316
77.371
77.160
76.949
37.655
21.540
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
N
Me
O
Ts
NH
9as
Filename = TK-6-136-1-2_carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-136-1-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-JUN-2024 22:54:24
Revision_Time = 24-JUN-2024 23:46:21
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 = 130
Total_Scans = 130
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 21.8[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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]

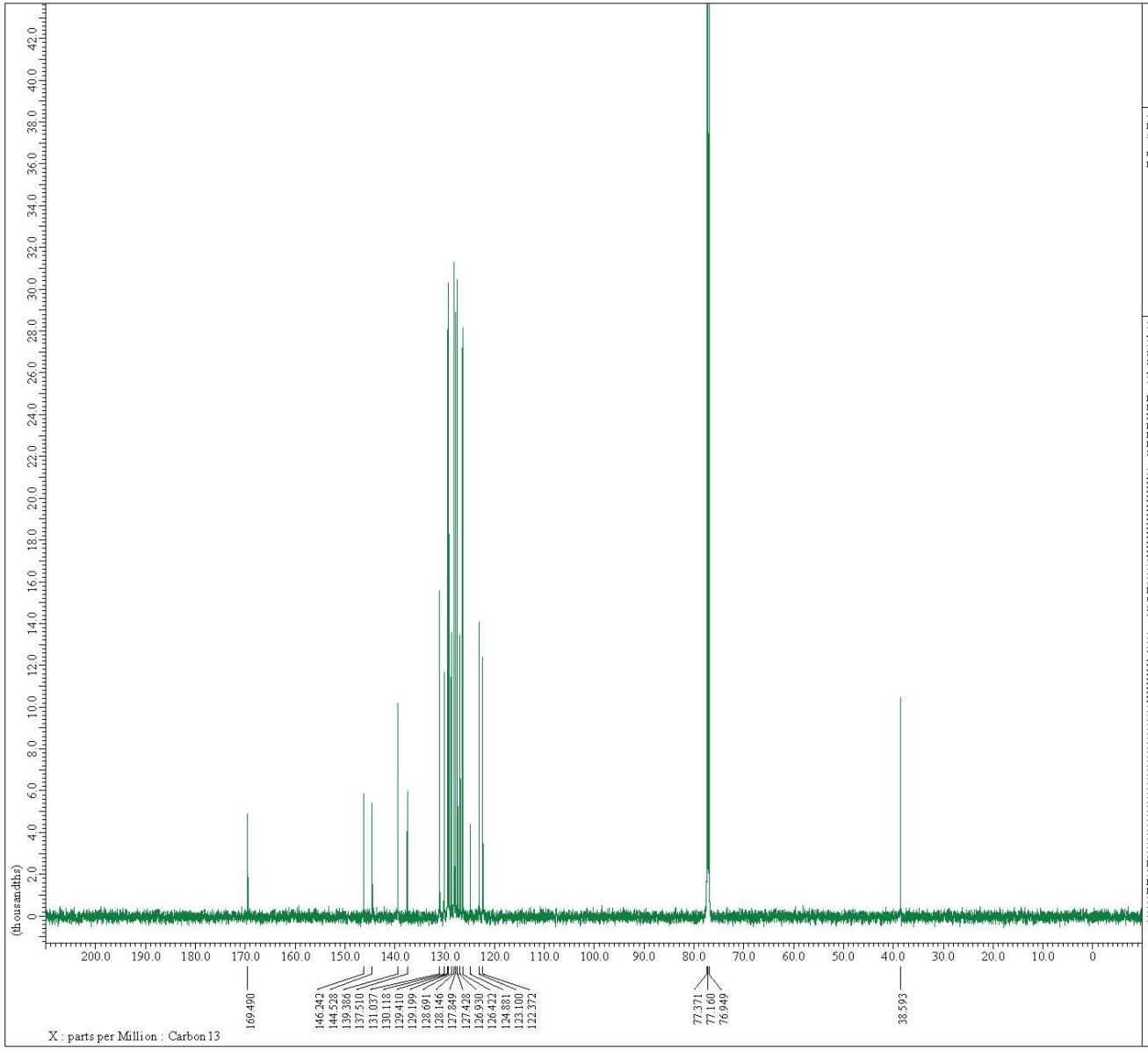


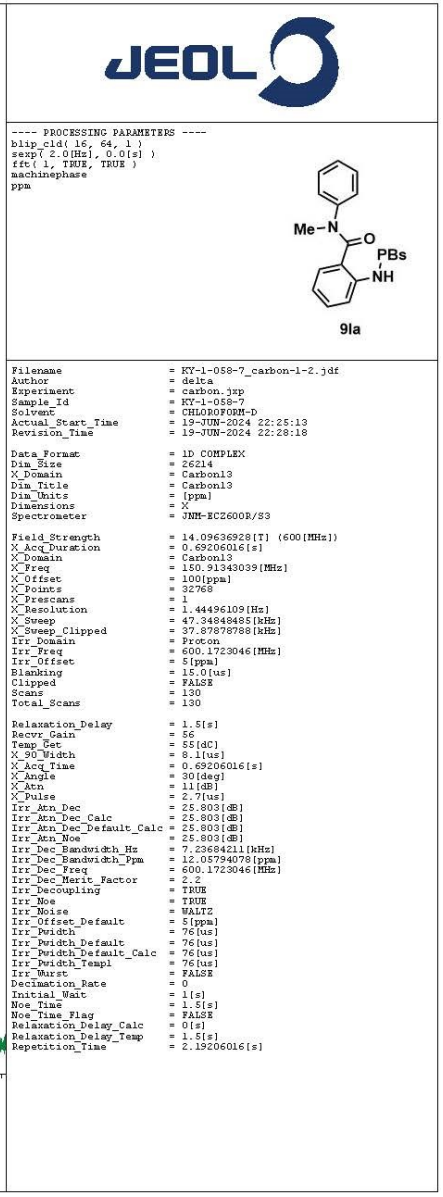


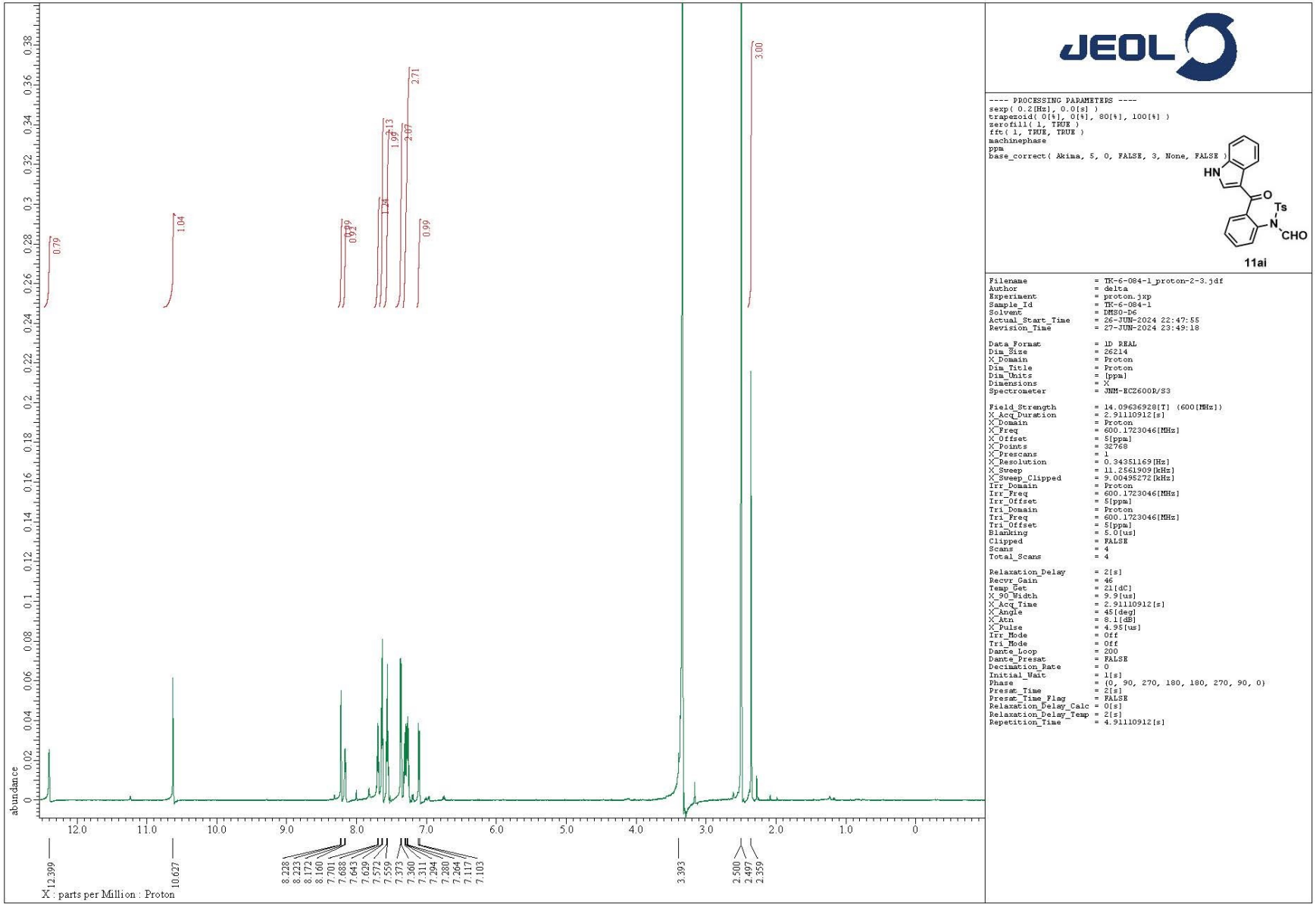

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.24864[ppm], 7.26[ppm] )
thresh( 3.47868[%], 1, )

以下に由来:: KY-1-058-7 proton-2-1.jdf
```

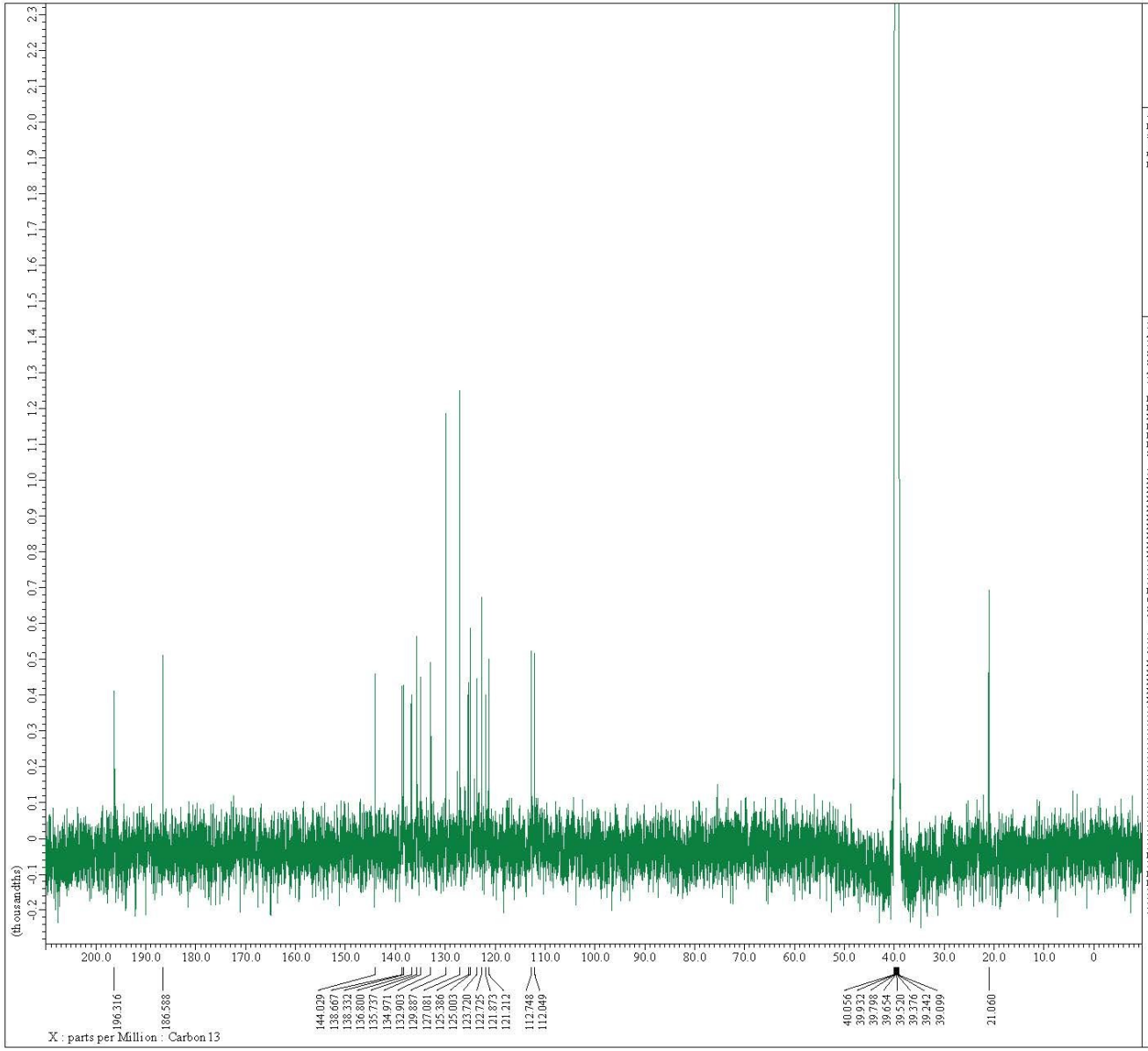

9la

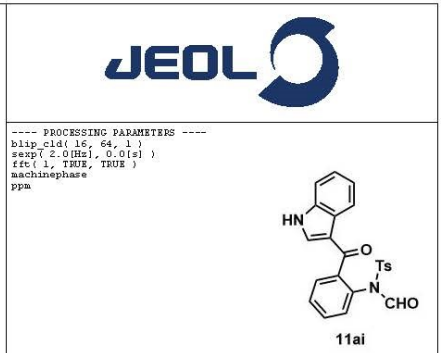
```
Filename                = KY-1-058-7_proton-2-2.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = KY-1-058-7
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 20-JUN-2024 22:42:37
Revision_Time           = 21-JUN-2024 08:01:03

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              = 46
Temp_Get                = 21.1[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```


(thousandths)
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
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
169.490
146.242
144.528
139.386
137.510
131.037
130.118
129.410
129.199
128.691
128.146
127.849
127.428
126.930
126.422
124.881
123.100
122.372
77.371
77.160
76.949
38.593
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
Me
N
O
PBs
NH
9la
Filename = KY-1-058-7_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = KY-1-058-7
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2024 22:25:13
Revision_Time = 19-JUN-2024 22:28:18
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 = 130
Total_Scans = 130
Relaxation_Delay = 1.5[s]
Recvr_Gain = 56
Temp_Get = 55[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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1.5[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1.5[s]
Repetition_Time = 2.19206016[s]


JEOL
---- 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, FALSE)
HN
O
Ts
N
CHO
11ai
Filename = TK-6-084-1_proton-2-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-084-1
Solvent = DMSO-D6
Actual_Start_Time = 26-JUN-2024 22:47:55
Revision_Time = 27-JUN-2024 23:49:18
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[MHz])
X_Acq_Duration = 2.91110912[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.34351169[Hz]
X_Sweep = 11.2561909[kHz]
X_Sweep_Clipped = 9.00495272[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 = 46
Temp_Set = 21[dC]
X_90_Width = 9.9[us]
X_Acq_Time = 2.91110912[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 = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.91110912[s]
abundance
0.79
1.04
0.99
1.24
2.13
1.99
2.07
2.71
0.99
3.00
12.399
10.627
8.228
8.223
8.172
8.160
7.701
7.688
7.643
7.629
7.572
7.559
7.373
7.360
7.311
7.294
7.280
7.264
7.117
7.103
3.393
2.500
2.497
2.359
X : parts per Million : Proton

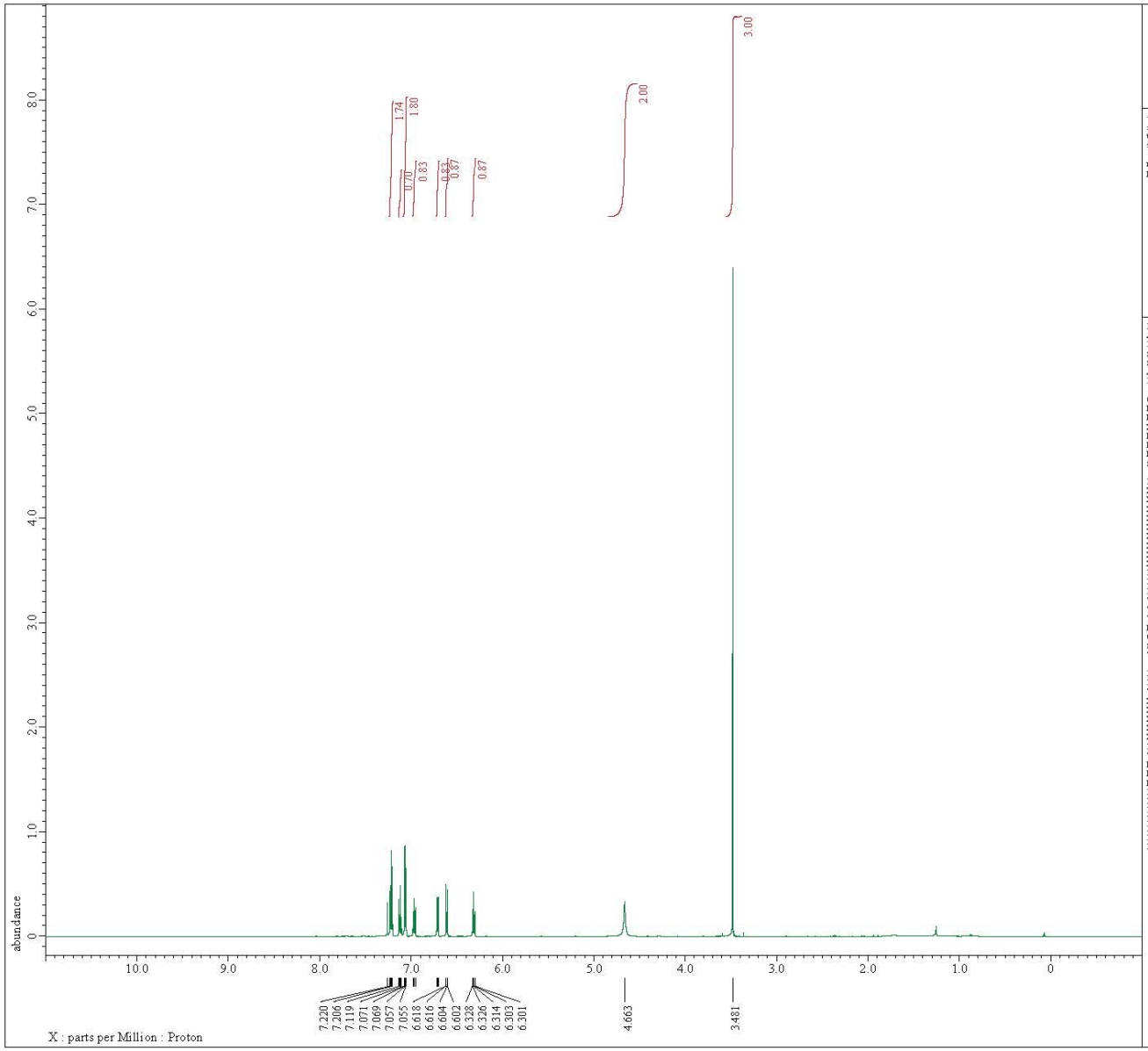


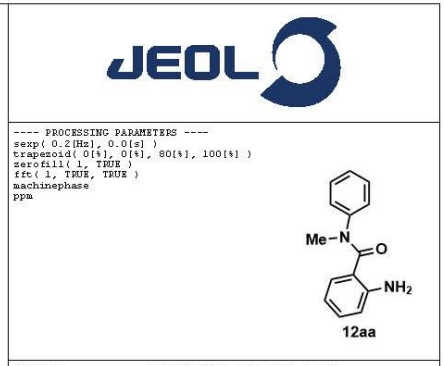



```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```


11ai

Filename	= TK-6-084-1-5_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-084-1-5
Solvent	= DMSO-D6
Actual_Start_Time	= 27-JUN-2024 21:58:13
Revision_Time	= 27-JUN-2024 23:13:37
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	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.6[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Declination_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

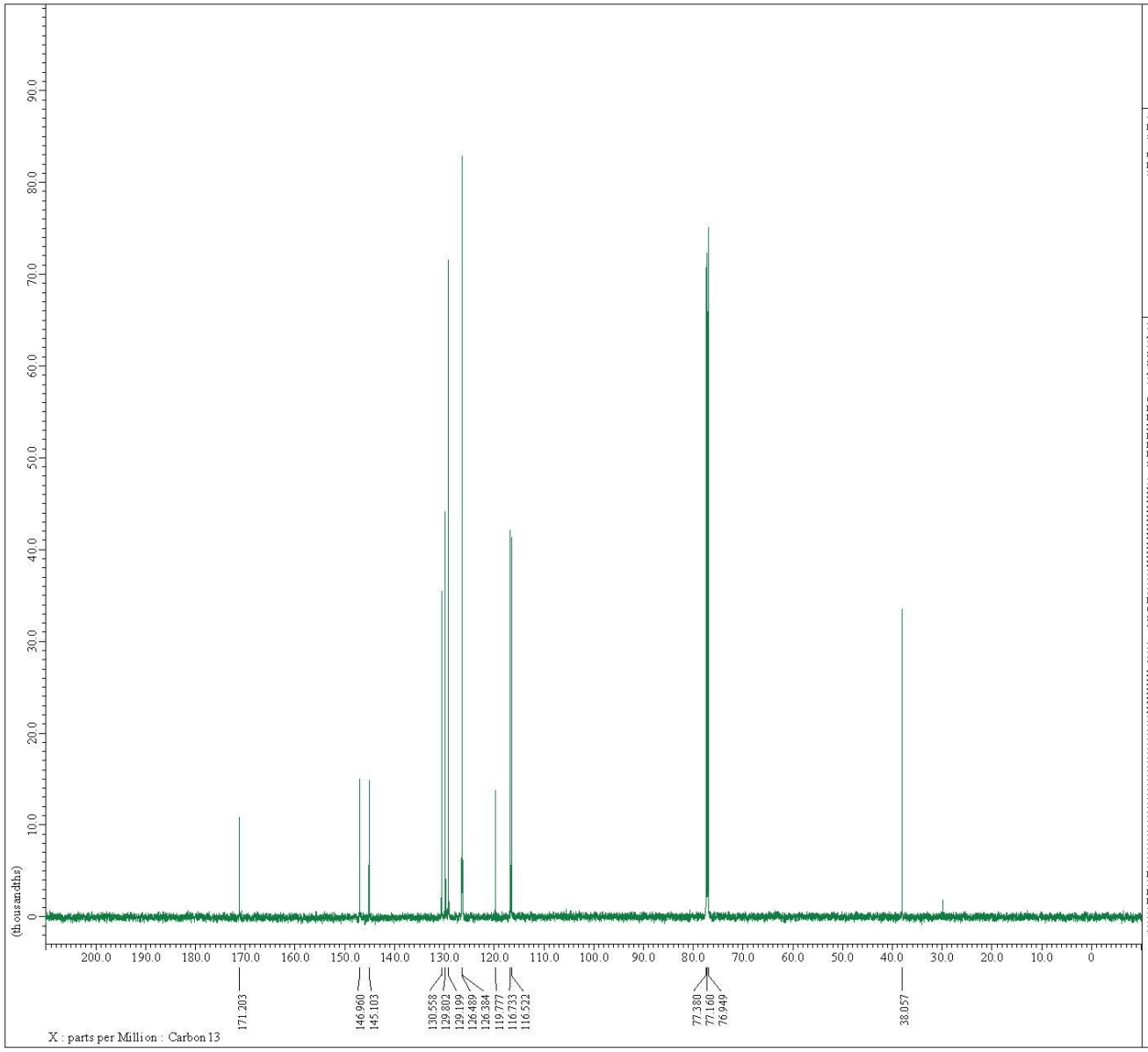


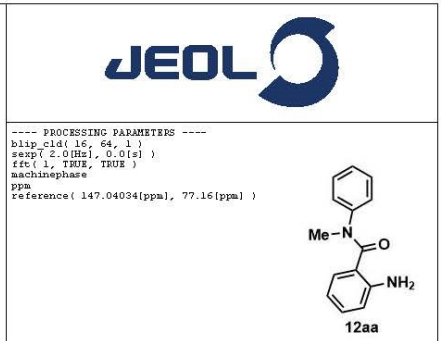



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```


12aa

```
Filename                = TK-6-028-2-1_proton-1-2.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TK-6-028-2-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  7-MAR-2024 22:36:16
Revision_Time           =  7-MAR-2024 22:38:47

Comment                 = single_pulse
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                = 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                   = 4
Total_Scans             = 4

Relaxation_Delay        = 2[s]
Recvr_Gain              = 36
Temp_Get                = 20.8[dC]
X_90_Width              = 9.9[us]
X_Acq_Time              = 2.18103808[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                   = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18103808[s]
```

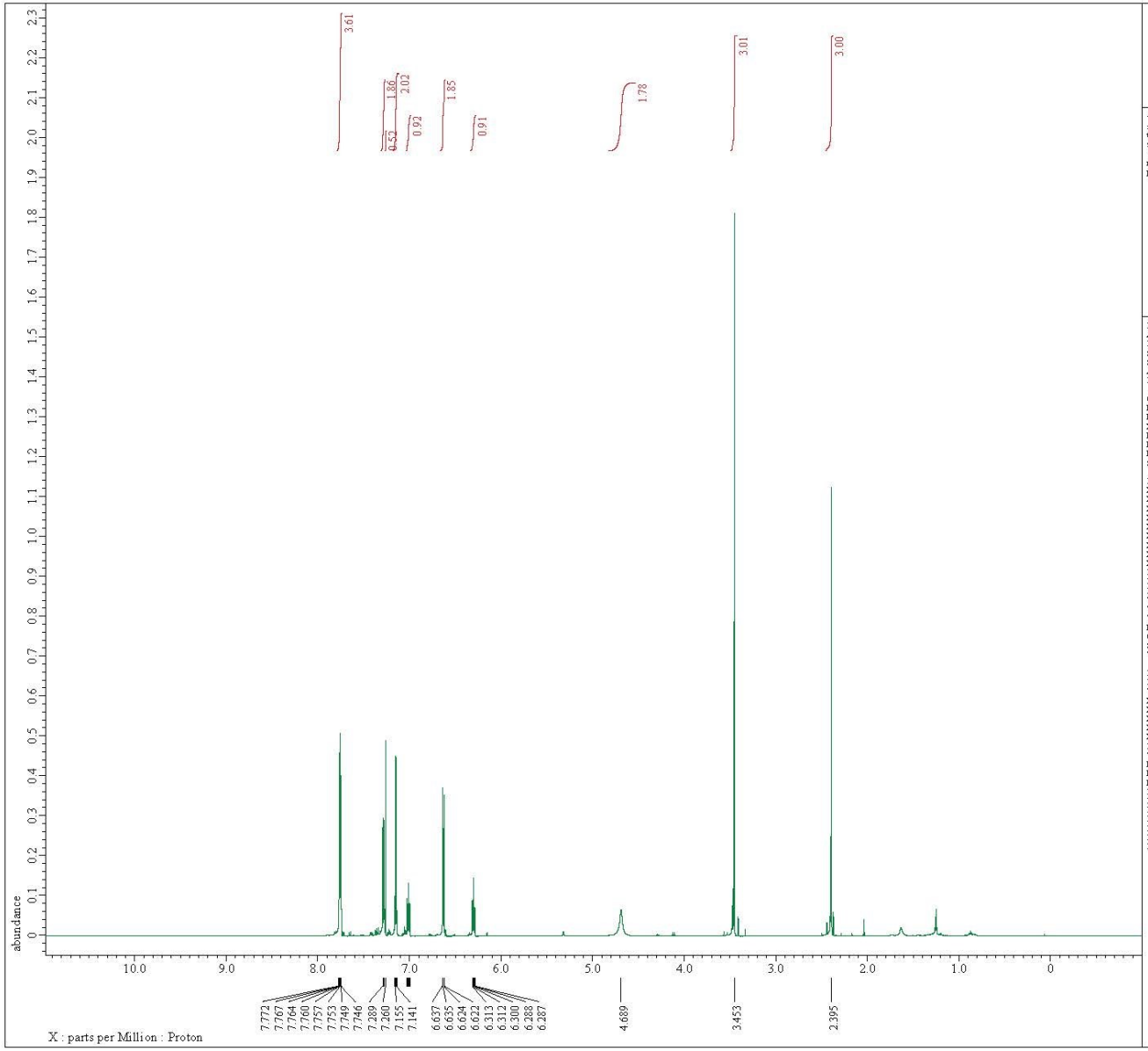


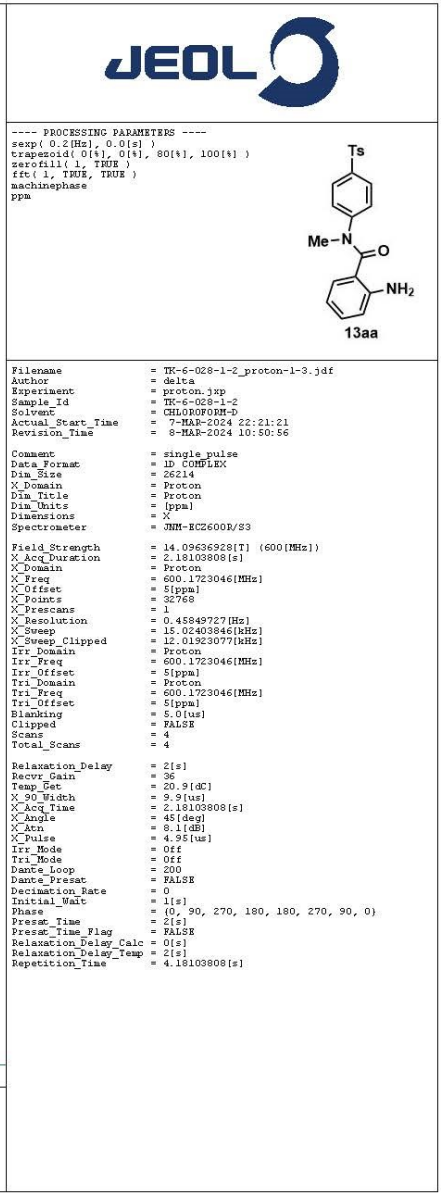


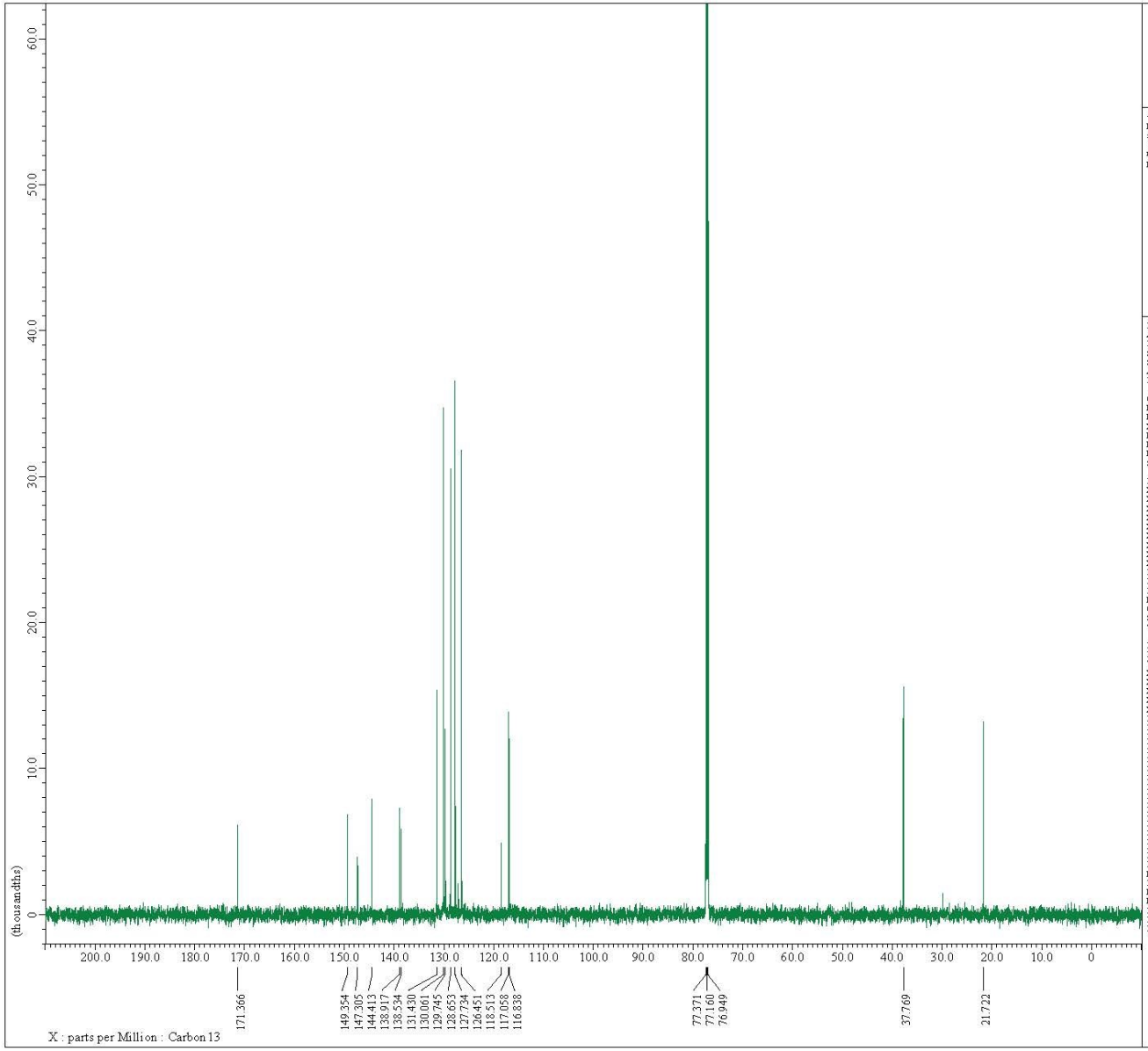

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
ffc( 1, TRUE, TRUE )
machinephase
ppm
reference( 147.04034[ppm], 77.16[ppm] )
```

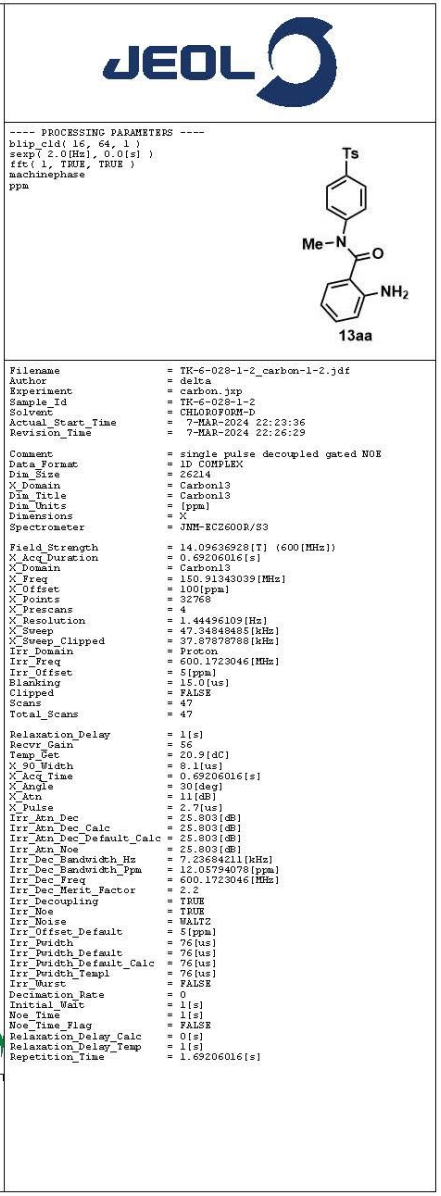

12aa

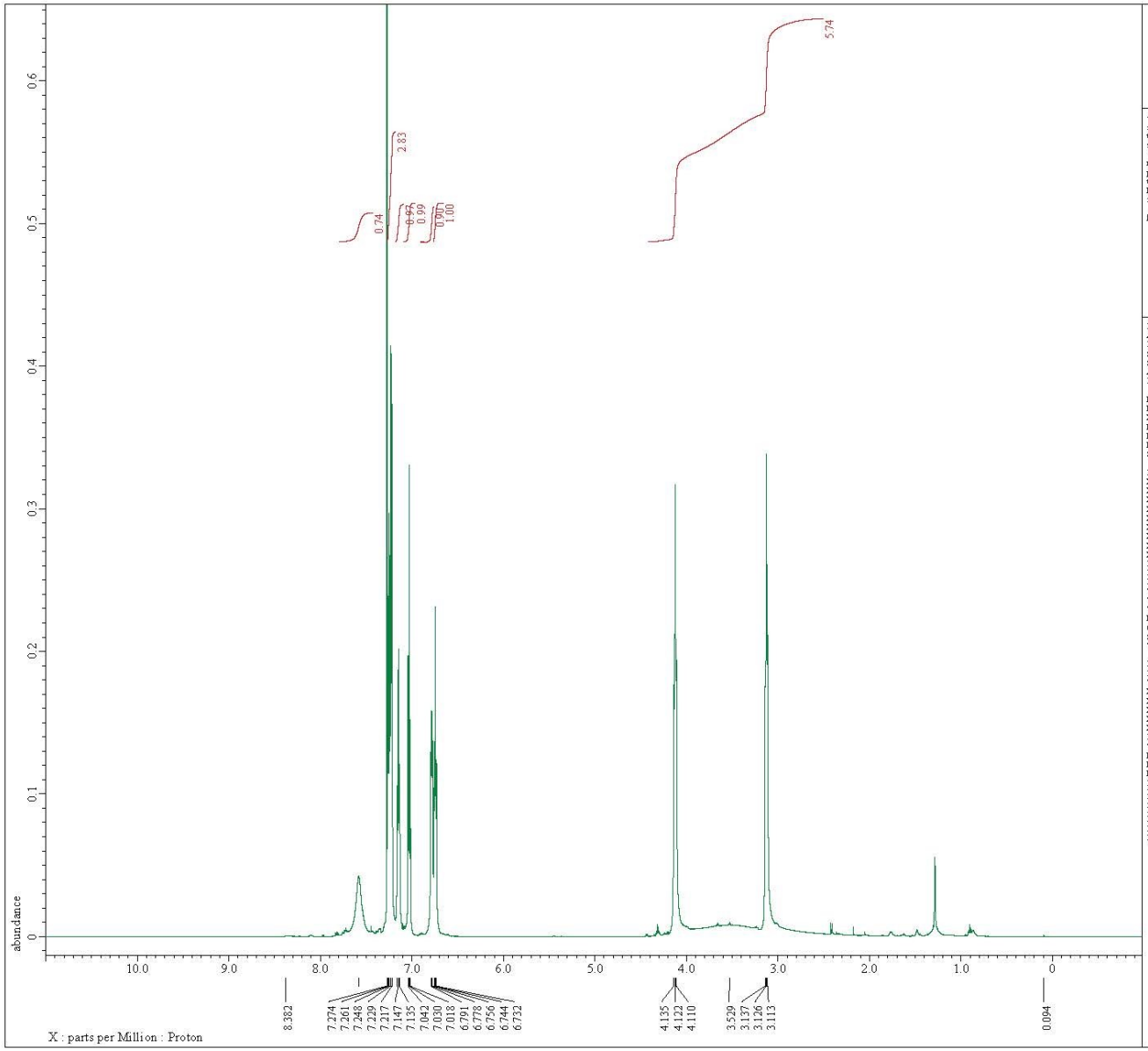
```
Filename                = TK-6-028-2-1_carbon-1-2.jdf
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = TK-6-028-2-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  7-MAR-2024 22:38:43
Revision_Time           =  7-MAR-2024 22:43:03

Comment                 = single pulse decoupled gated NOE
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                   = 64
Total_Scans             = 64

Relaxation_Delay        = 1[s]
Recvr_Gain              = 56
Temp_Get                = 20.8[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_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 76[us]
Irr_Pwidth_Default      = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ        = 76[us]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Noe_Time                = 1[s]
Noe_Time_Flag           = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 1[s]
Repetition_Time         = 1.69206016[s]
```


3.61
1.86
2.02
0.53
0.92
1.85
0.91
1.78
3.01
3.00
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.772
7.767
7.764
7.760
7.757
7.753
7.749
7.746
7.289
7.260
7.155
7.141
6.637
6.635
6.624
6.622
6.313
6.312
6.300
6.288
6.287
4.689
3.453
2.395
X : parts per Million : Proton


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Ts
Me–N
O
NH2
13aa
Filename = TK-6-028-1-2_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-028-1-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-MAR-2024 22:21:21
Revision_Time = 8-MAR-2024 10:50:56
Comment = single_pulse
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 = 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 = 4
Total_Scans = 4
Relaxation_Delay = 2[s]
Recvr_Gain = 36
Temp_Get = 20.9[dC]
X_90_Width = 9.9[us]
X_Acq_Time = 2.18103808[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 = {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18103808[s]

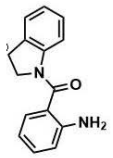

(thousandths)
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
171.366
149.354
147.305
144.413
138.917
138.534
131.430
130.061
129.745
128.653
127.734
126.451
118.513
117.058
116.838
77.371
77.160
76.949
37.769
21.722
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
Ts
Me–N
O
NH2
13aa
Filename = TK-6-028-1-2_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-028-1-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-MAR-2024 22:23:36
Revision_Time = 7-MAR-2024 22:26:29
Comment = single pulse decoupled gated NOE
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 = 47
Total_Scans = 47
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_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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]



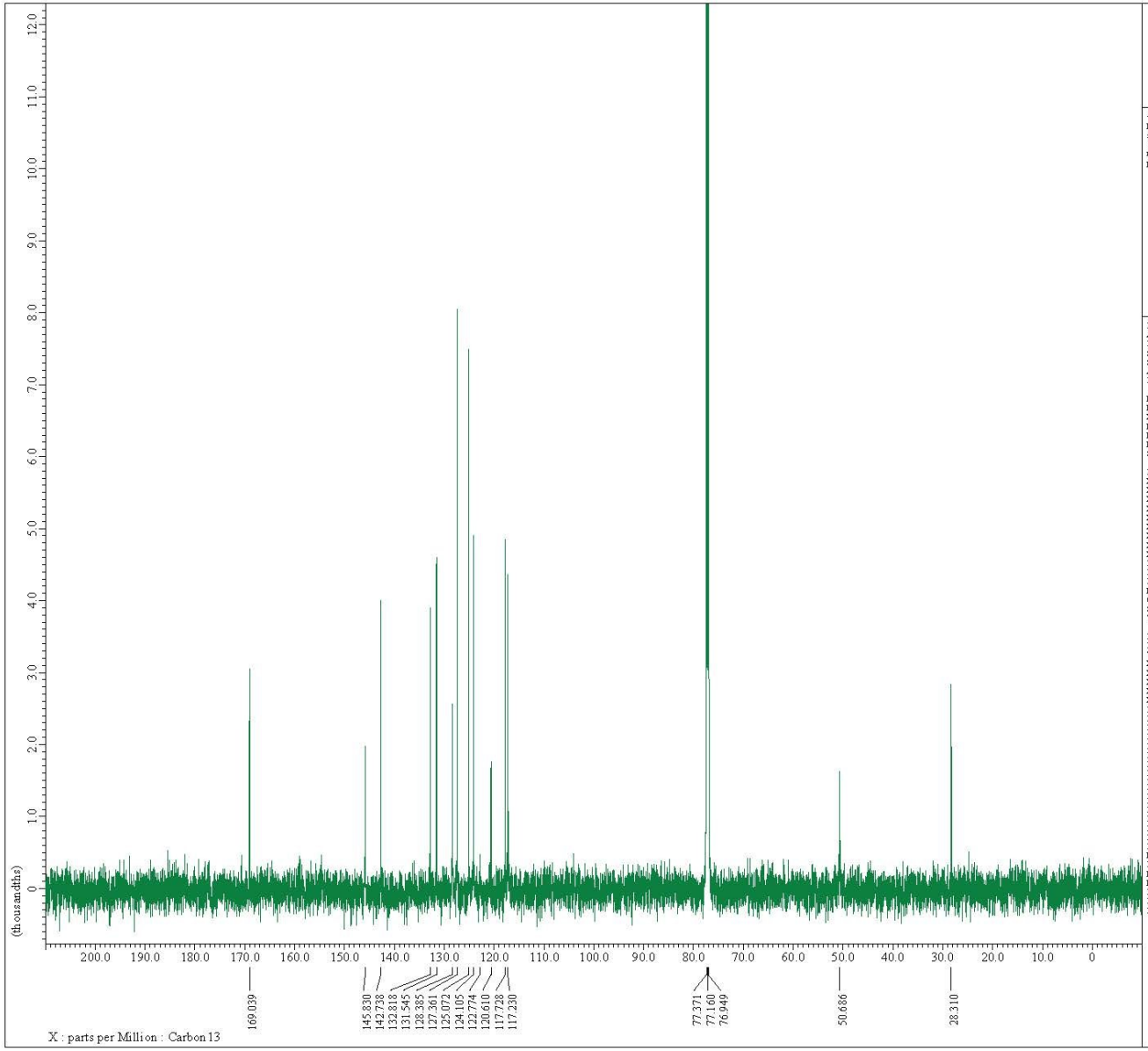
JEOL

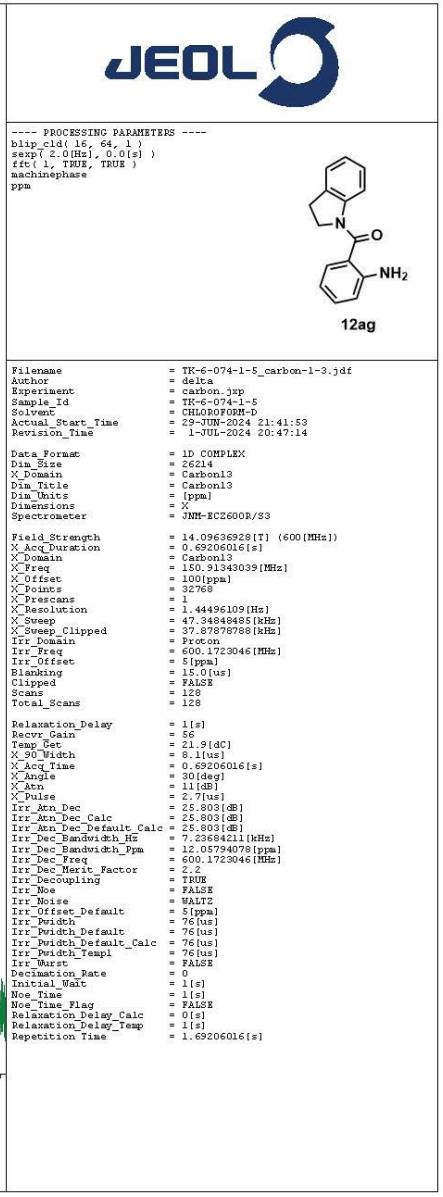
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 0.93356[%], 1,  )
base_correct( Akima, 5, 0, FALSE, 3, None, FALSE )
reference( 7.24635[ppm], 7.26[ppm] )

以下由来:: TK-6-074-1-5 proton-2-1.jdf
```

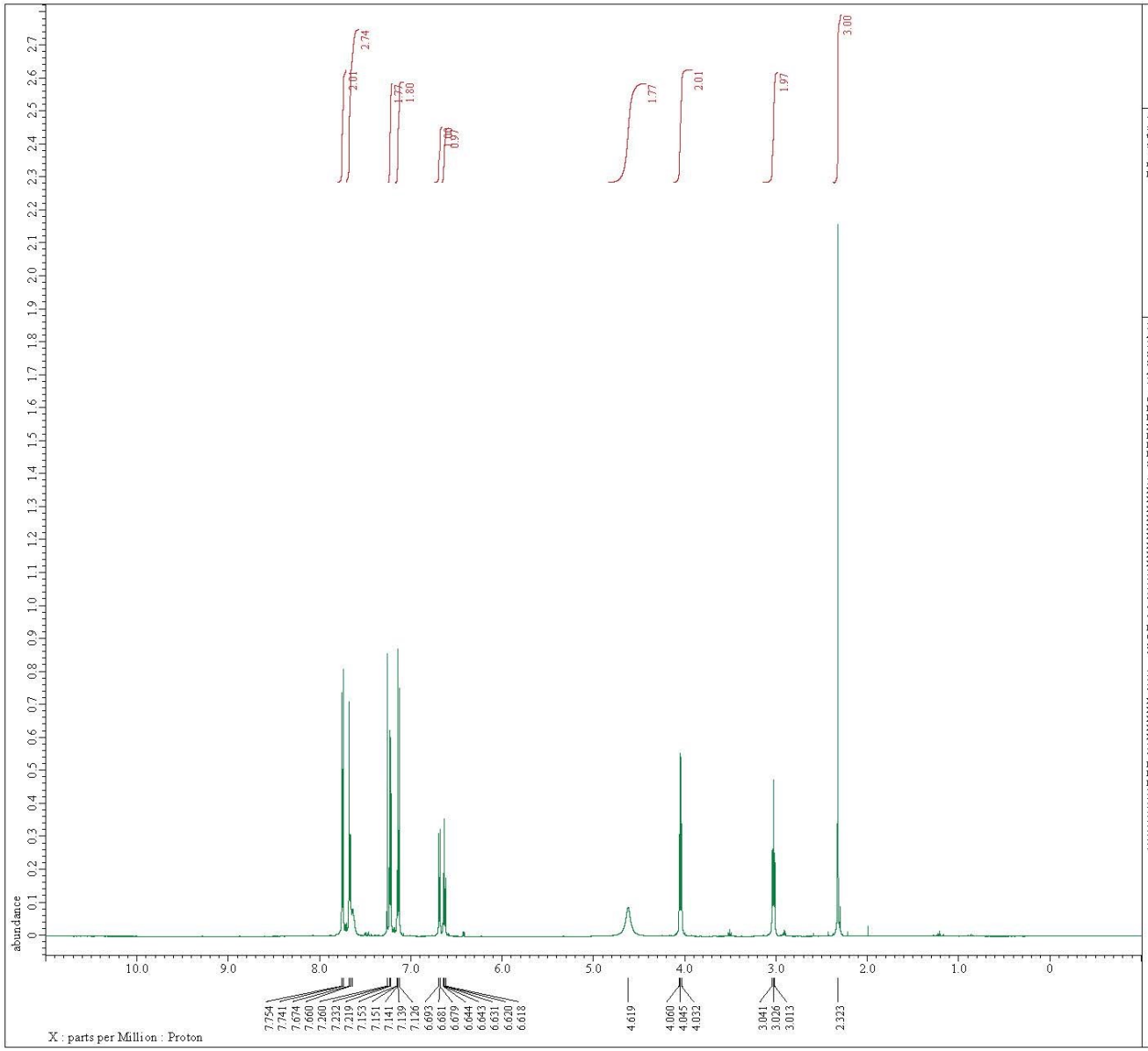


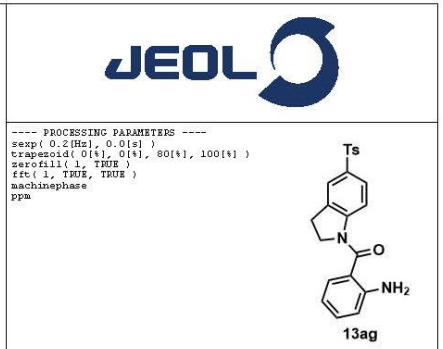
12ag

Filename	= TK-6-074-1-5_proton-2-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-6-074-1-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JUN-2024 22:38:22
Revision_Time	= 1-JUL-2024 20:52:20
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[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	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 46
Temp_Get	= 45[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	= {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.18365952[s]


(thousandths)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
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
169.039
145.830
143.738
132.818
131.545
128.385
127.361
125.072
124.105
122.774
120.610
117.728
117.230
77.371
77.160
76.949
50.686
28.310
X : parts per Million : Carbon13

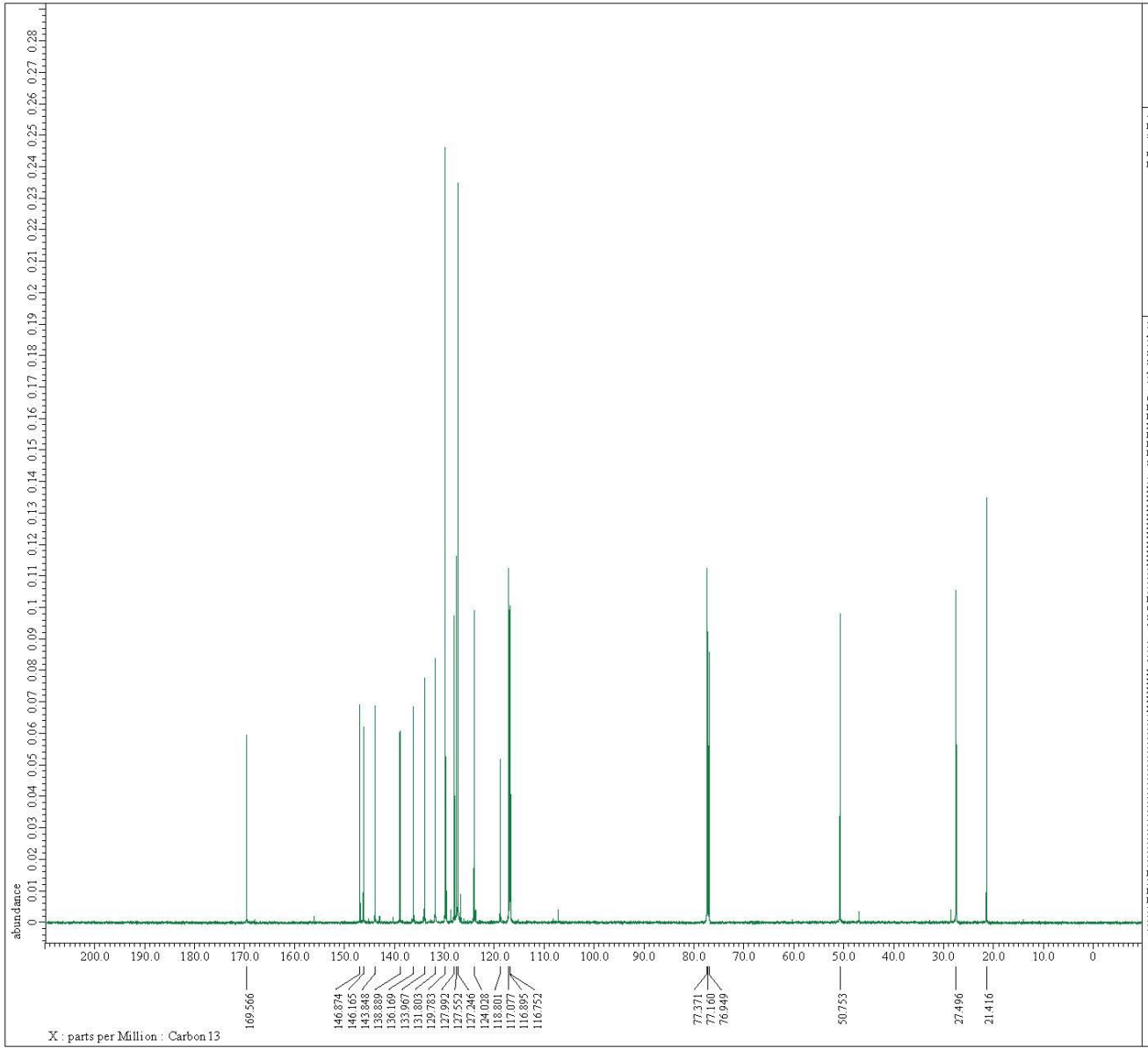

JEOL
---- PROCESSING PARAMETERS ----
blip_cld(16, 64, 1)
sexp(2.0[Hz], 0.0[s])
fft(1, TRUE, TRUE)
machinephase
ppm
N
O
NH2
12ag
Filename = TK-6-074-1-5_carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-074-1-5
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JUN-2024 21:41:53
Revision_Time = 1-JUL-2024 20:47:14
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 = 150.91343039[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 = 128
Total_Scans = 128
Relaxation_Delay = 1[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_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = FALSE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time = 1.69206016[s]

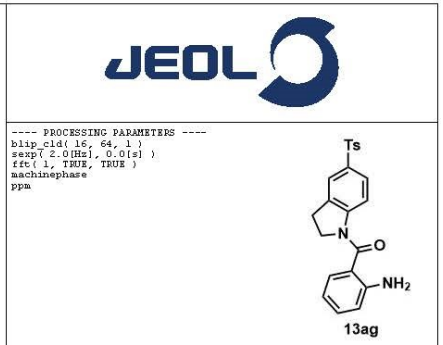





```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

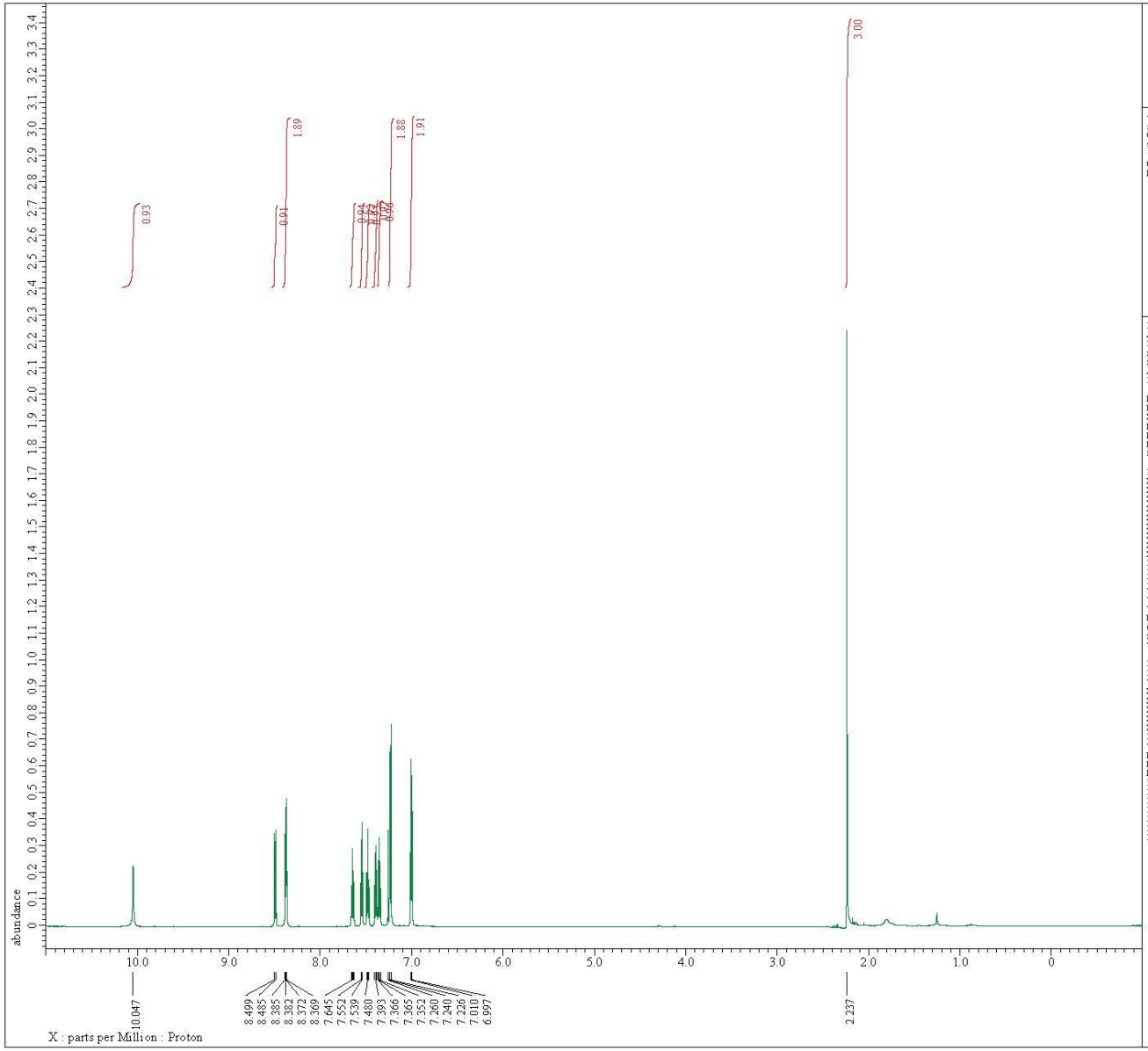
Filename	= TK-6-094-2_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-6-094-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-APR-2024 16:39:18
Revision_Time	= 24-APR-2024 18:28:56
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
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	= 21.6[dC]
X_90_Width	= 9.9[us]
X_Acq_Time	= 2.90455552[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	= {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.90455552[s]

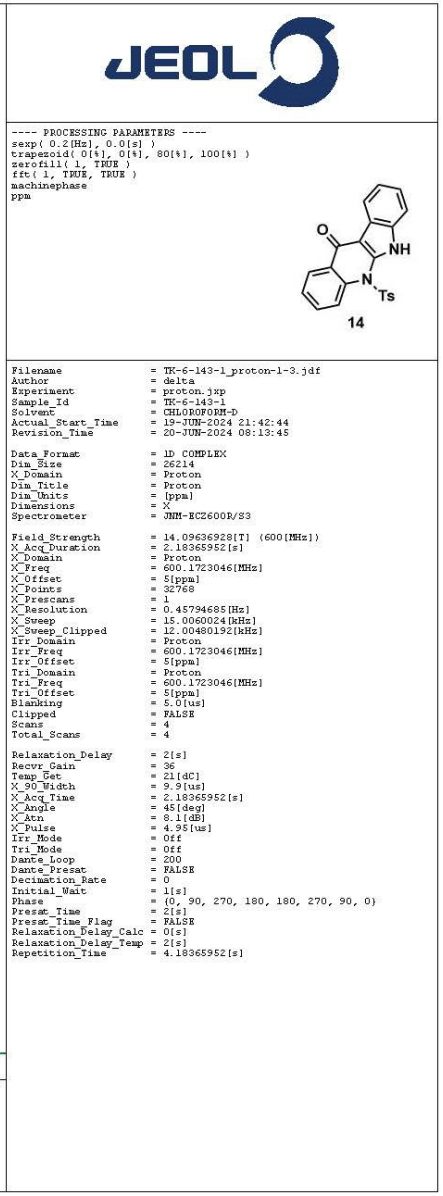


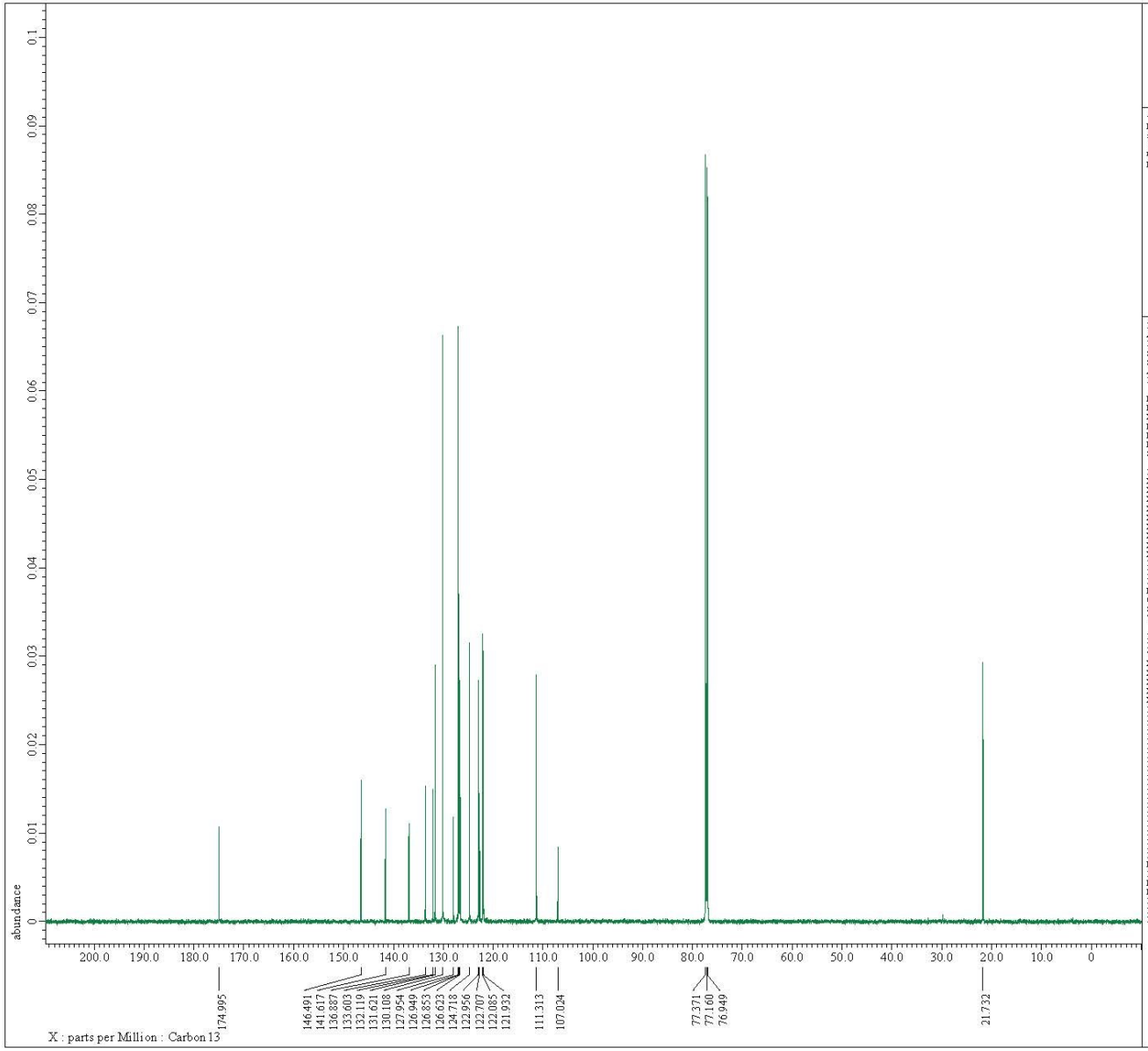


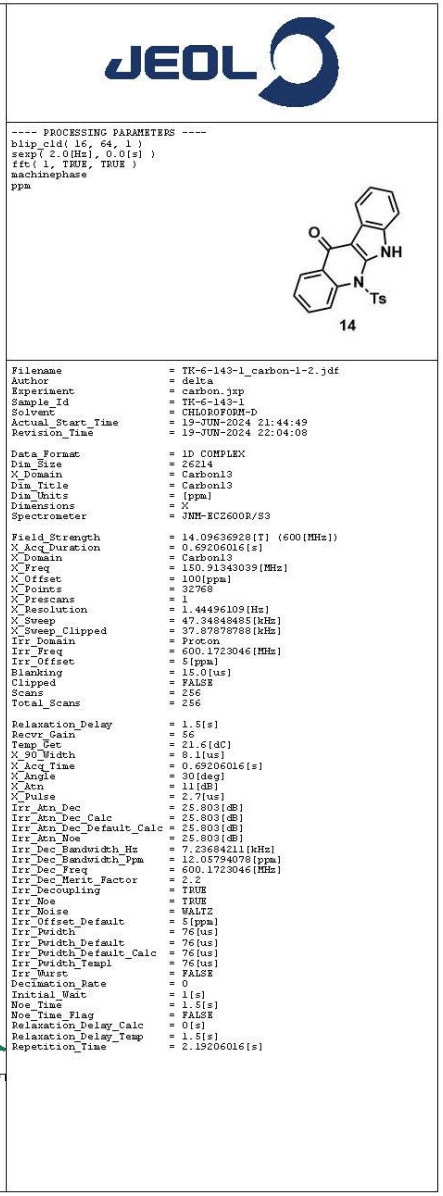

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

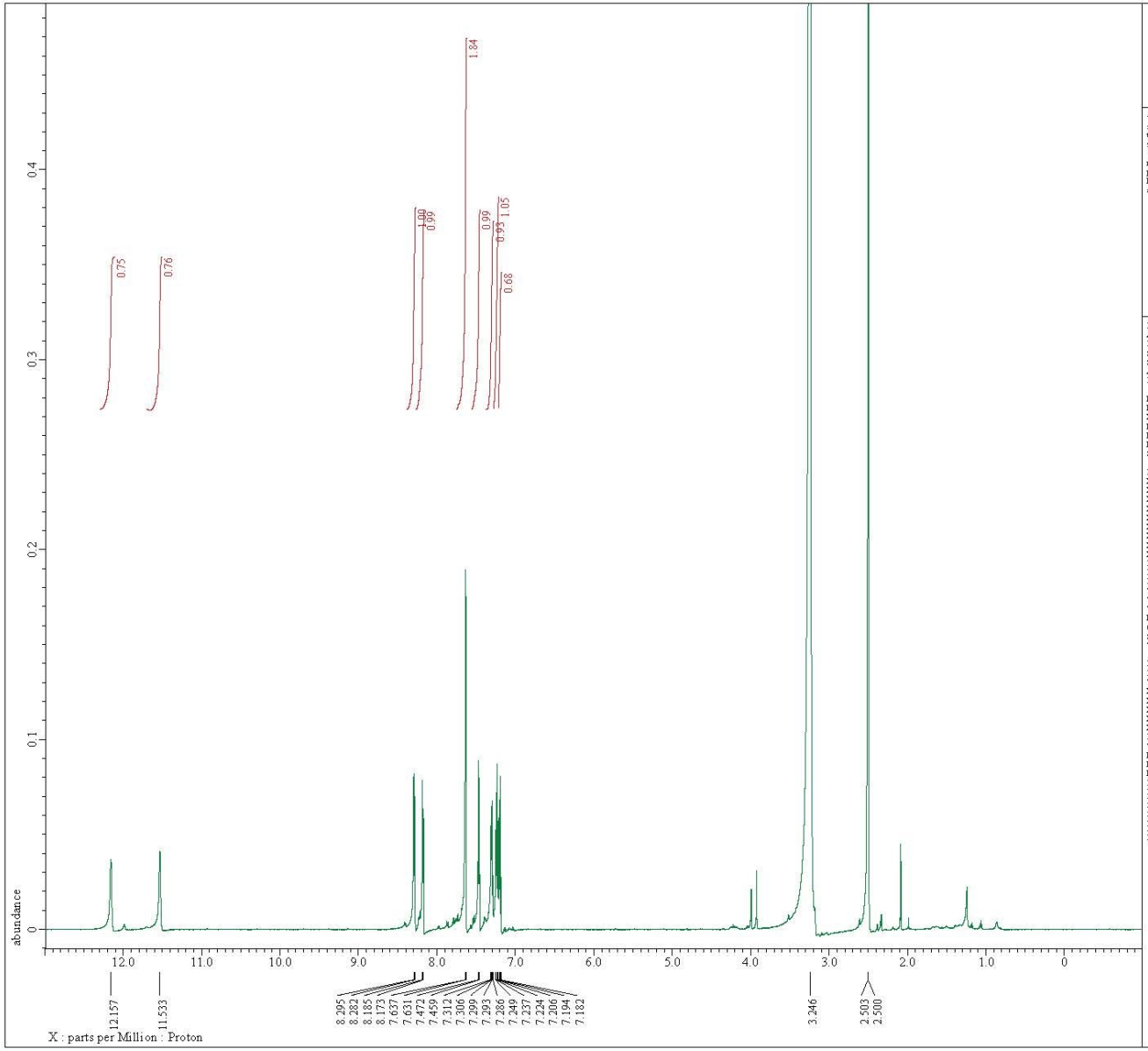
Filename	= TK-6-094-2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-094-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-APR-2024 16:40:15
Revision_Time	= 24-APR-2024 16:46:55
Comment	= single pulse decoupled gated NOE
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
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	= 172
Total_Scans	= 172
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 22[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_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]


abundance
X : parts per Million : Proton
10.047
8.499
8.485
8.385
8.382
8.372
8.369
7.645
7.552
7.539
7.480
7.393
7.366
7.365
7.352
7.260
7.240
7.226
7.010
6.997
2.237
0.93
1.89
0.91
1.88
1.91
3.00


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
O
NH
N
Ts
14
Filename = TK-6-143-1_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = TK-6-143-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2024 21:42:44
Revision_Time = 20-JUN-2024 08:13:45
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 = 36
Temp_Set = 21[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 = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18365952[s]

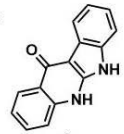

abundance
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
174.995
146.491
141.617
136.887
133.603
132.119
131.621
130.108
127.954
126.949
126.853
126.623
124.718
122.956
122.707
122.085
121.932
111.313
107.024
77.371
77.160
76.949
21.732
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
O
NH
N
Ts
14
Filename = TK-6-143-1_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-6-143-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUN-2024 21:44:49
Revision_Time = 19-JUN-2024 22:04:08
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 = 256
Total_Scans = 256
Relaxation_Delay = 1.5[s]
Recvr_Gain = 56
Temp_Get = 21.6[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_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Templ = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 1.5[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1.5[s]
Repetition_Time = 2.19206016[s]



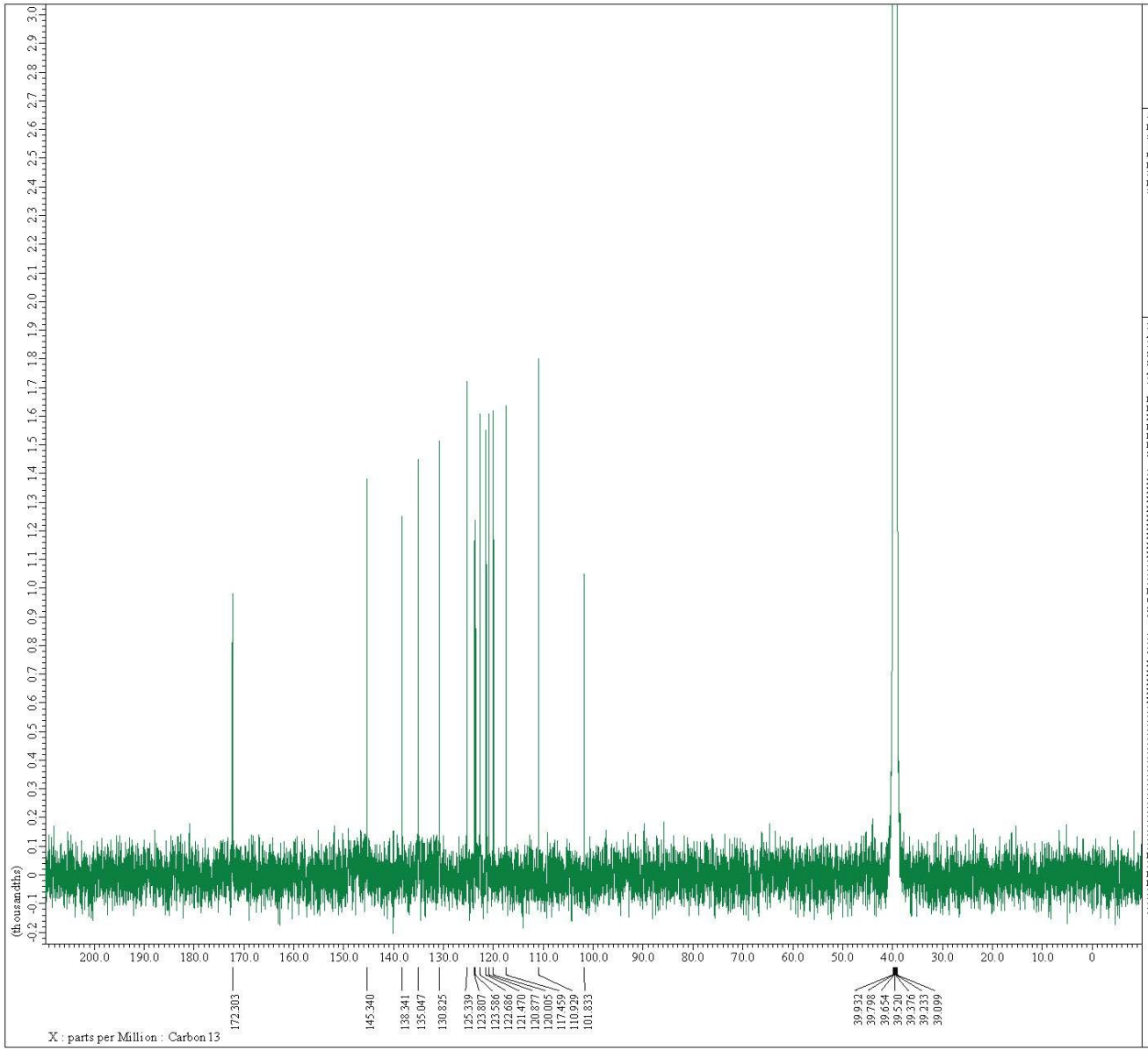
JEOL

```
---- 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, FA
auto_phase( 10[%], FALSE, 0[Hz], 0[Hz] )
```



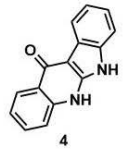
4

```
Filename                = Tk-6-146-1-7_proton-2-3.jdf
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = Tk-6-146-1-7
Solvent                 = DMSO-D6
Actual_Start_Time       = 29-JUN-2024 21:36:34
Revision_Time           =  3-JUL-2024 14:13:35

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[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                   = 8
Total_Scans             = 8

Relaxation_Delay        = 2[s]
Recvr_Gain              = 46
Temp_Set                = 50[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                   = (0, 90, 270, 180, 180, 270, 90, 0)
Presat_Time             = 2[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 2[s]
Repetition_Time         = 4.18365952[s]
```



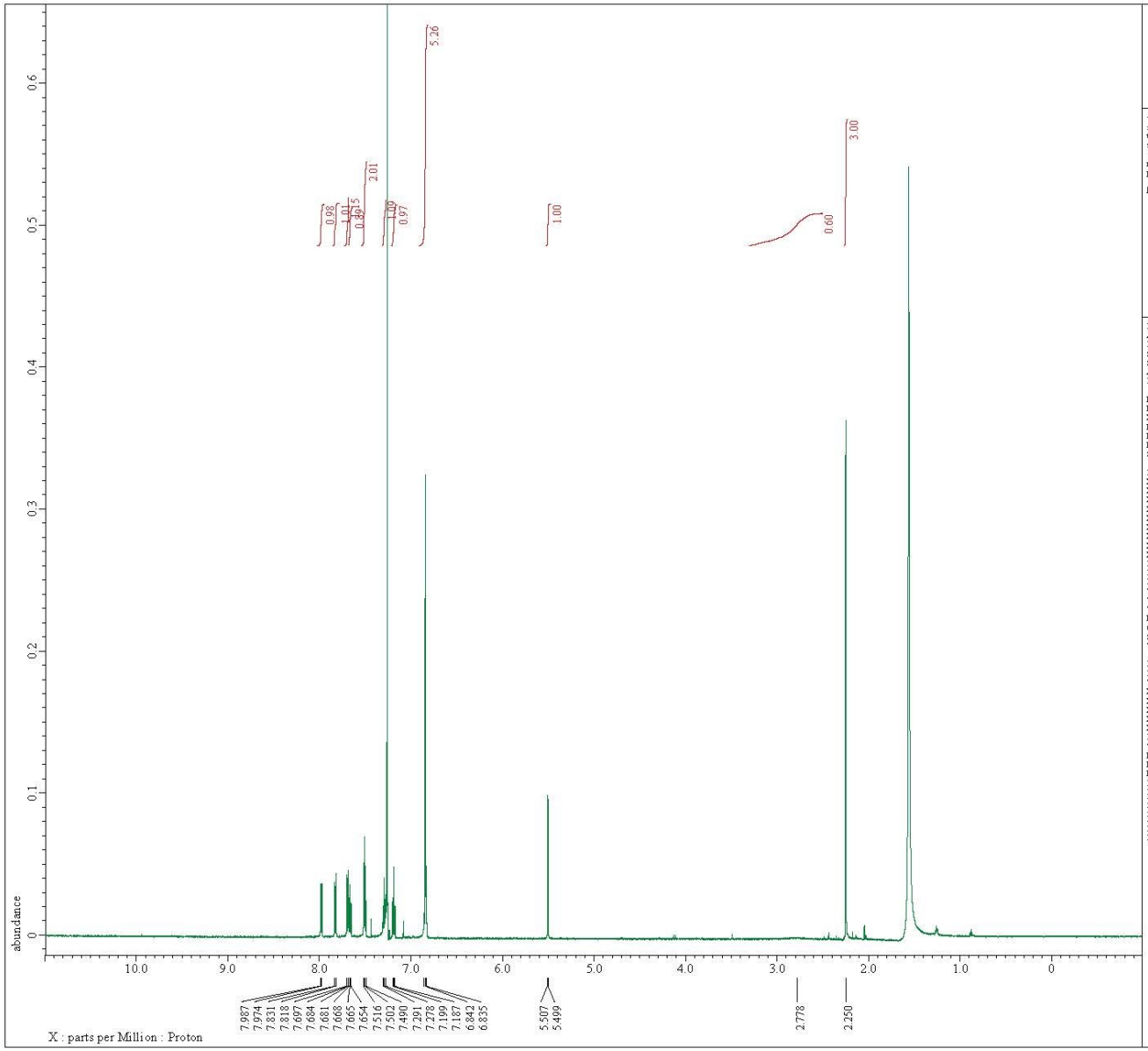
JEOL

```
---- PROCESSING PARAMETERS ----
blip_cld( 16, 64, 1 )
sexp( 2.0[Hz], 0.0[s] )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 40.01408[ppm], 39.52[ppm] )
phase( -0.25, 0, 20[%] )
ibase_correct( , FALSE, FALSE, FALSE )
```



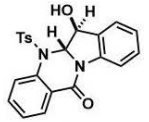
4

Filename	= TK-6-146-1-7_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-146-1-7
Solvent	= DMSO-D6
Actual_Start_Time	= 28-JUN-2024 22:09:17
Revision_Time	= 28-JUN-2024 22:58:51
Data_Format	= 1D REAL
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	= TRUE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 21[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



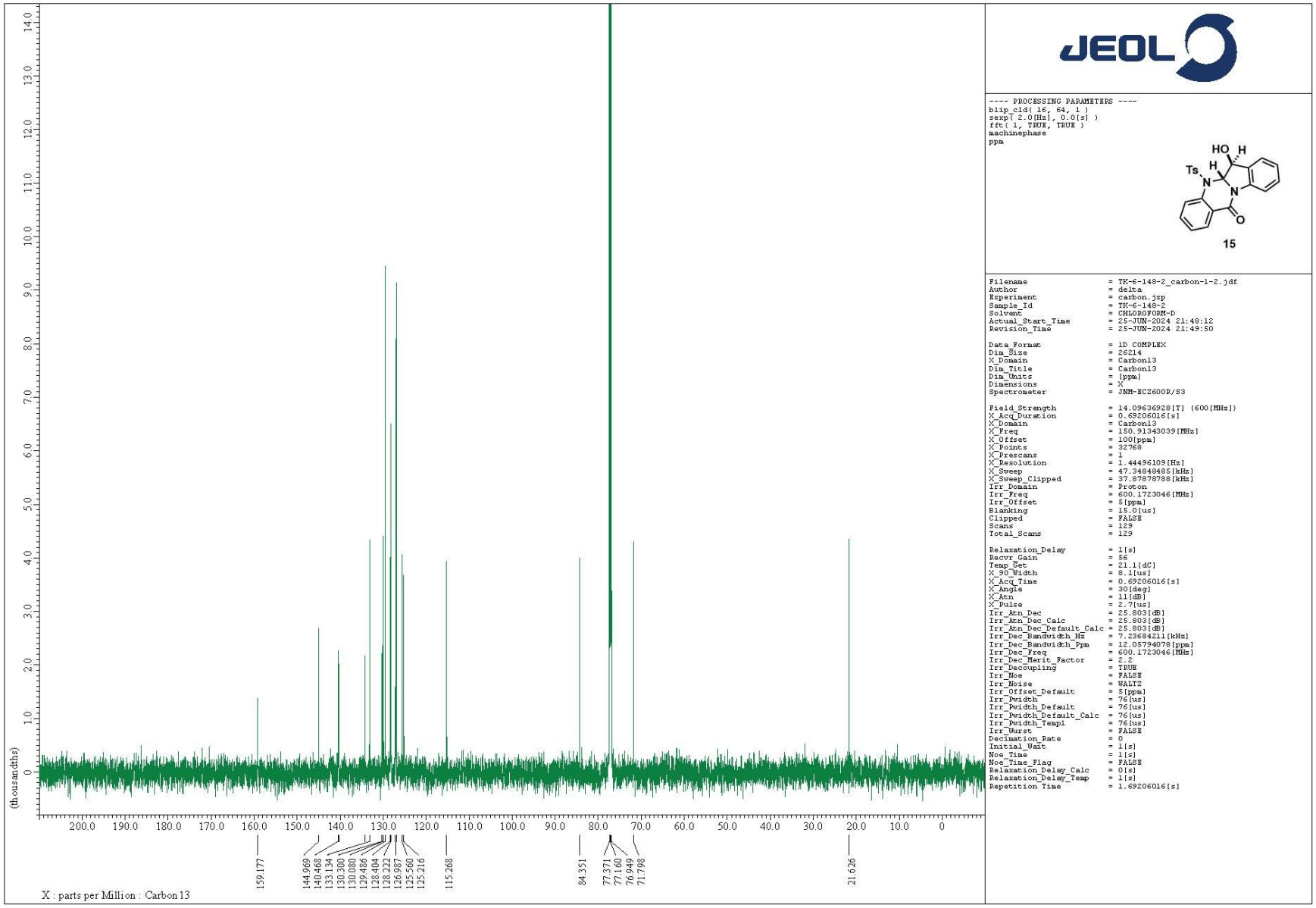
JEOL

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

以下由来:: TK-6-148-2-2_proton-1-1.jdf
```



15

Filename	= TK-6-148-2-2_proton-1-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TK-6-148-2-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-JUN-2024 22:06:07
Revision_Time	= 3-JUL-2024 14:47:21
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	= 2.91110912[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.34351169[Hz]
X_Sweep	= 11.2561909[kHz]
X_Sweep_Clipped	= 9.00495272[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	= 56
Temp_Get	= 21[dC]
X_90_Width	= 9.9[us]
X_Acq_Time	= 2.91110912[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	= {0, 90, 270, 180, 180, 270, 90, 0}
Presat_Time	= 2[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 4.91110912[s]



JEOL

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


15

Filename	= TK-6-148-2_carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TK-6-148-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2024 21:48:12
Revision_Time	= 25-JUN-2024 21:49:50
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	= 129
Total_Scans	= 129
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Set	= 21.1[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_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]