

Revisiting 3-Azidoindoles: Overcoming A Trade-Off Challenges Between Stability and Reactivity in Utilization of in situ-Generated Azidoindoles

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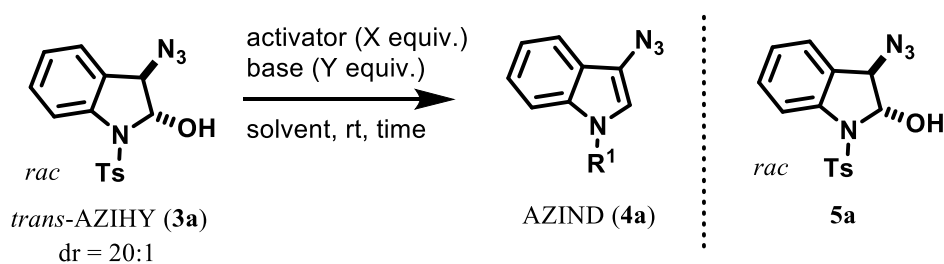
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Supporting Information

General methods	S2
Optimization of reaction conditions (Table S1)	S3
Experimental procedures and spectra data for obtained products	S4–S25
References	S26
¹ H and ¹³ C NMR spectra	S27–S90

General methods. Column chromatography was carried out using silica gel (WAKO Gel 75–150 mesh, WAKO Co., Ltd.). Preparative thin-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) values, and coupling constants are expressed in hertz (Hz). ^1H NMR spectra were referenced to a solvent signal (CDCl_3 : 7.26 ppm, $\text{DMSO}-d_6$: 2.50 ppm and acetone- d_6 : 2.05 ppm). ^{13}C NMR spectra were referenced to a solvent signal (CDCl_3 : 77.1 ppm, $\text{DMSO}-d_6$: 39.5 ppm and acetone- d_6 : 29.8 ppm). 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), broad (br). High-resolution MS spectra were recorded with a Bruker 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

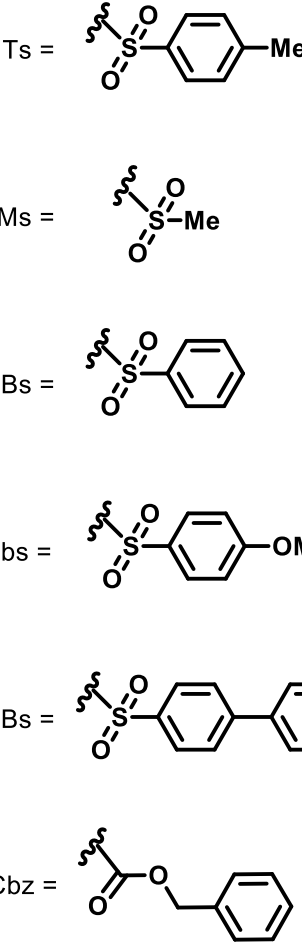


Run	Activator (X equiv.)	Base (Y equiv.)	solvent	time (h)	Yield (%) of 4a ^b
1	MsCl (1.5)	KOt-Bu (2.0)	THF	24	19
2	MsCl (1.5)	Pyridine (2.0)	THF	24	7
3	MsCl (1.5)	DIPEA (2.0)	THF	24	70
4	MsCl (1.5)	DBU (2.0)	THF	15 min	24
5	MsCl (1.5)	Et₃N (2.0)	THF	15 min	91
6	TsCl (1.5)	Et ₃ N (2.0)	THF	24	61
7	TsCl (1.5)	Pyridine (2.0)	THF	24	3
8	Ac ₂ O (1.5)	Et ₃ N (2.0)	THF	24	0 ^c
9	MsCl (1.5)	Et ₃ N (2.0)	MeCN	24	70
10	MsCl (1.5)	Et ₃ N (2.0)	toluene	24	84
11	MsCl (1.5)	Et ₃ N (2.0)	AcOEt	15 min	81
12	MsCl (1.5)	Et ₃ N (3.0)	THF	15 min	84
13	MsCl (1.1)	Et₃N (2.0)	THF	15 min	90
14	MsCl (1.1)	Et ₃ N (1.5)	THF	24	61
15	MsCl (1.1)	Et ₃ N (1.1)	THF	24	67
16	-	Et ₃ N (2.0)	THF	24	0
17	MsCl (1.5)	-	THF	24	nr

^a Reaction conditions: **3a** (0.5 mmol), **activator** (0.5 × X mmol), and **base** (0.5 × Y mmol) in solvent (2.5 mL) under air at room temperature.; ^b Isolated yield.; ^c O-Ac-AZIH **5a** was obtained in 78% yield.

Synthesis of *N*-protected indoles S1

The *N*-protected indoles **S1** as *N*-tosylindoles (**S1a**, **S1g–S1n**), *N*-methanesulfonylindole (**S1b**), *N*-benzenesulfonylindole (**S1c**), *N*-(4-methoxybenzenesulfonyl)indole (**S1d**), *N*-(4-phenylbenzenesulfonyl)indole (**S1e**) and *N*-benzyloxycarbonylindole (**S1f**) were prepared by reported method.^[1] 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.^[1]

<i>N</i>-protected indoles	S1a : ($R^1 = \text{Ts}$, $R^2 = \text{H}$)	
	S1b : ($R^1 = \text{Ms}$, $R^2 = \text{H}$)	
	S1c : ($R^1 = \text{Bs}$, $R^2 = \text{H}$)	
	S1d : ($R^1 = \text{Mbs}$, $R^2 = \text{H}$)	
	S1e : ($R^1 = \text{PhBs}$, $R^2 = \text{H}$)	
	S1f : ($R^1 = \text{Cbz}$, $R^2 = \text{H}$)	
	S1g : ($R^1 = \text{Ts}$, $R^2 = 5\text{-MeO}$)	
	S1h : ($R^1 = \text{Ts}$, $R^2 = 5\text{-Me}$)	
	S1i : ($R^1 = \text{Ts}$, $R^2 = 5\text{-Cl}$)	
	S1j : ($R^1 = \text{Ts}$, $R^2 = 5\text{-Br}$)	
	S1k : ($R^1 = \text{Ts}$, $R^2 = 6\text{-Cl}$)	
	S1l : ($R^1 = \text{Ts}$, $R^2 = 4\text{-Cl}$)	
	S1m : ($R^1 = \text{Ts}$, $R^2 = 7\text{-Cl}$)	
	S1n : ($R^1 = \text{Ts}$, $R^2 = 7\text{-aza}$)	

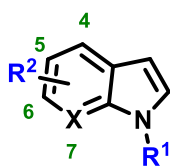


Figure S1.

Synthesis of *trans*-3-azido-2-hydroxyindolines (AZIHYS) **3**

The *trans*-3-azido-2-hydroxyindolines (AZIHYS) **3** were prepared by reported method [2]. All reagents were weighed and handled in air at room temperature. Analytical data are in accordance with the literature values (**3a**, **3b**, **3g**, **3h**, **3i**, **3j**, **3k**, **3l** and **3n** [2]).

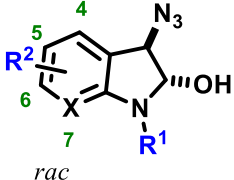
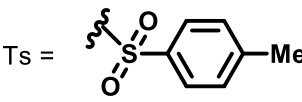
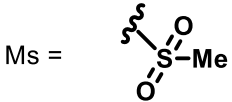
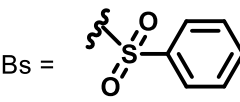
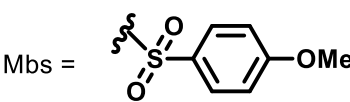
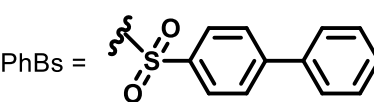
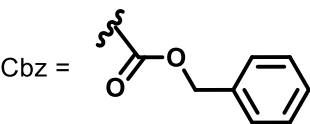
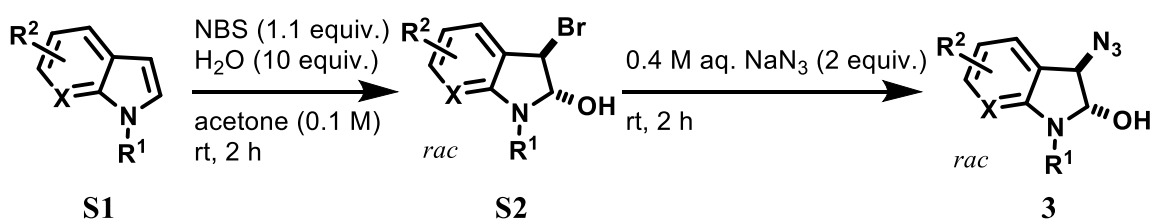
	N-protected AZIHYS	3a : (R ¹ = Ts, R ² = H)	
		3b : (R ¹ = Ms, R ² = H)	
		3c : (R ¹ = Bs, R ² = H)	
		3d : (R ¹ = Mbs, R ² = H)	
		3e : (R ¹ = PhBs, R ² = H)	
		3f : (R ¹ = Cbz, R ² = H)	
		3g : (R ¹ = Ts, R ² = 5-MeO)	
		3h : (R ¹ = Ts, R ² = 5-Me)	
		3i : (R ¹ = Ts, R ² = 5-Cl)	
		3j : (R ¹ = Ts, R ² = 5-Br)	
		3k : (R ¹ = Ts, R ² = 6-Cl)	
		3l : (R ¹ = Ts, R ² = 4-Cl)	
		3m : (R ¹ = Ts, R ² = 7-Cl)	
		3n : (R ¹ = Ts, R ² = 7-aza)	
			     

Figure S2.

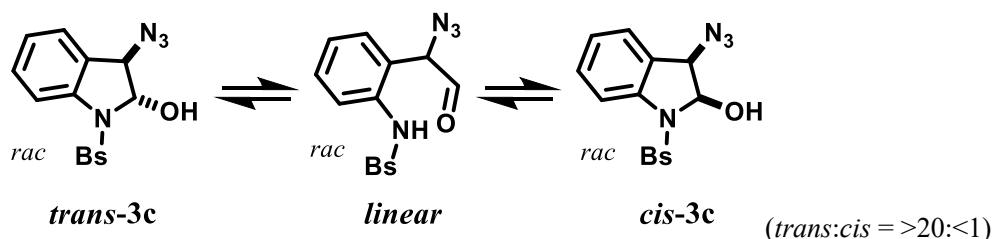
General procedure A



To a solution of *N*-protected indole **S1** (5 mmol) and H₂O (0.90 mL, 10 equiv., 50 mmol) in acetone (25 mL, 0.5 M) was added NBS (979 mg, 1.1 equiv., 5.5 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material indicated by TLC. Then, 0.4 M aq. NaN₃ (25 mL, 2 equiv.) was

added to the mixture. After the mixture was stirred for a further 2 h, the whole was extracted with AcOEt (3 × 50 mL). The combined organic layer was washed with brine (50 mL), dried over Na₂SO₄, filtered and concentrated *in vacuo*. The residue was purified by silica gel column chromatography to give **3**.

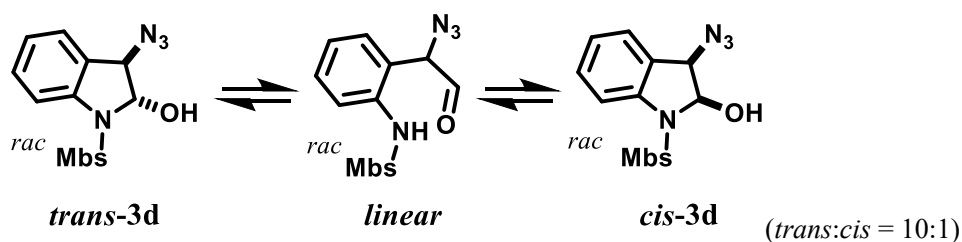
***trans*-3-Azido-1-(phenylsulfonyl)indolin-2-ol (**3c**)**



The reaction was performed according to the general procedure A using 1.29 g (5.0 mmol) of **S1c**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **3c** (1.80 g, 4.1 mmol, 91% yield) as a white solid.

White solid (1.80 g, 4.1 mmol, 91% yield; mp 91–93 °C); IR (KBr) ν : 3465, 3077, 2962, 2096, 1344, 1164, 723 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 7.84 (d, *J* = 7.8 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.41 (td, *J* = 7.8, 1.2 Hz, 1H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.15 (td, *J* = 7.8, 1.2 Hz, 1H), 5.58 (dd, *J* = 2.4, 1.2 Hz, 1H), 4.59 (s, 1H), 3.47 (d, *J* = 3.6 Hz, 1H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 140.7, 1378, 134.0, 131.3, 129.5, 127.0, 126.3, 125.9, 124.8, 115.1, 91.3, 66.4; HRMS (ESI) *m/z*: [M+Na]⁺ Calcd for C₁₄H₁₂N₄O₃SNa 339.0528; Found 339.0524.

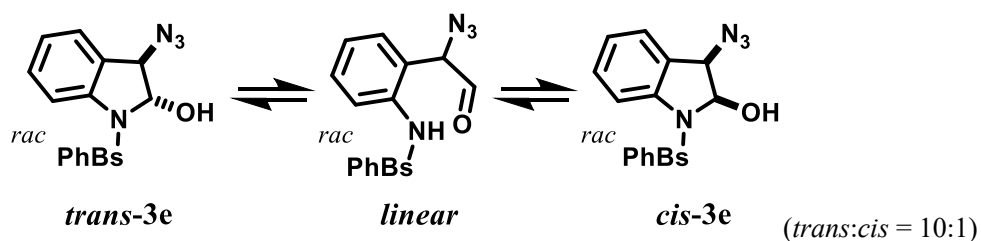
***trans*-3-Azido-1-((4-methoxyphenyl)sulfonyl)indolin-2-ol (**3d**)**



The reaction was performed according to the general procedure A using 1.44 g (5.0 mmol) of **S1d**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **3d** (1.46 g, 4.21 mmol, 84% yield) as a white solid.

White solid (1.46 g, 4.21 mmol, 84% yield; mp 94–96 °C); IR (KBr) ν : 3183, 3010, 2971, 2942, 2840, 2100, 1592, 1496, 1359, 1265, 1157, 755 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 7.77 (d, *J* = 9.0 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.39 (td, *J* = 7.2, 0.6 Hz, 1H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.13 (td, *J* = 7.8, 1.2 Hz, 1H), 6.91 (d, *J* = 9.0 Hz, 2H), 5.57 (dd, *J* = 3.6, 1.8 Hz, 1H), 4.59 (s, 1H), 3.81 (s, 3H), 3.53 (d, *J* = 3.6 Hz, 1H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 163.9, 140.8, 131.2, 129.30, 129.27, 126.2, 125.9, 124.6, 115.0, 114.7, 91.3, 66.5, 55.8; HRMS (ESI) *m/z*: [M+Na]⁺ Calcd for C₁₅H₁₄N₄O₄SNa 369.0633; Found 369.0634.

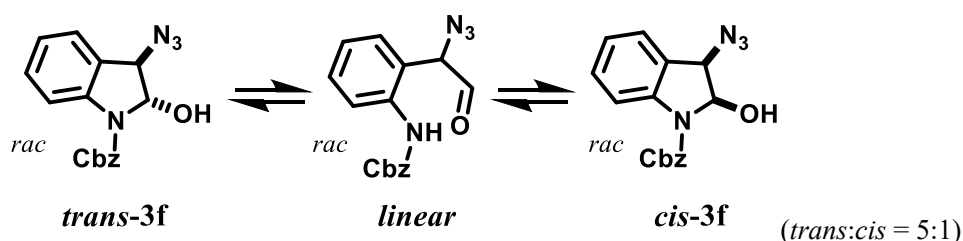
***trans*-1-([1,1'-Biphenyl]-4-ylsulfonyl)-3-azidoindolin-2-ol (**3e**)**



The reaction was performed according to the general procedure A using 1.67 g (5.0 mmol) of **S1e**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **3e** (1.35 g, 3.43 mmol, 69% yield) as a pale-yellow oil.

Pale-yellow oil (1.35 g, 3.43 mmol, 69% yield); IR (KBr) ν : 3467, 3068, 3031, 2100, 1355, 1166, 761 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.89 (d, J = 8.4 Hz, 2H), 7.69–7.65 (m, 3H), 7.53 (d, J = 7.2 Hz, 2H), 7.46–7.38 (m, 4H), 7.33 (dd, J = 7.2, 0.6 Hz, 1H), 7.16 (td, J = 7.8, 1.2 Hz, 1H), 5.64 (d, J = 1.8 Hz, 1H), 4.60 (s, 1H), 3.76 (s, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 146.9, 140.7, 139.1, 136.2, 131.3, 129.2, 128.8, 128.1, 127.5, 127.4, 126.3, 126.0, 124.8, 115.3, 91.3, 66.4; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{20}\text{H}_{16}\text{N}_4\text{O}_3\text{SNa}$ 415.0841; Found 415.0845.

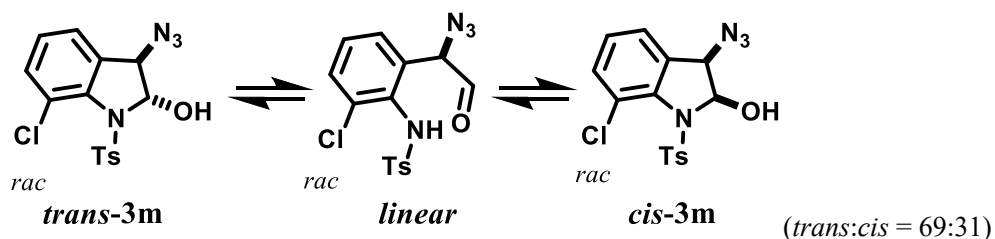
***trans*-Benzyl-3-azido-2-hydroxyindoline-1-carboxylate (**3f**)**



The reaction was performed according to the general procedure A using 1.26 g (5.0 mmol) of **S1f**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **3f** (1.11 g, 3.56 mmol, 71% yield) as an orange oil.

Orange oil (1.11 g, 3.56 mmol, 71% yield); IR (KBr) ν : 3448, 3066, 3033, 2960, 2102, 1712, 1482, 752 cm^{-1} ; ^1H NMR (600 MHz, acetone- d_6) δ 7.84 (br s, 1H), 7.52 (d, J = 7.2 Hz, 0.8H), 7.49 (d, J = 7.8 Hz, 2H), 7.42–7.32 (m, 5.2H), 7.14 (t, J = 7.8 Hz, 0.8H), 7.02 (t, J = 7.2 Hz, 0.2H), 6.09–6.07 (m, 0.4H), 5.92 (s, 0.8H), 5.74 (s, 0.8H), 5.38 (d, J = 12.6 Hz, 0.8H), 5.37 (d, J = 12.6 Hz, 0.2H), 5.28–5.26 (m, 1H), 4.85 (d, J = 6.0 Hz, 0.2H), 4.78 (s, 0.8H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, acetone- d_6) δ 1137.5, 132.0, 131.4, 130.4, 129.4, 129.0, 128.9, 126.9, 125.4, 124.0, 116.1, 88.9, 68.0, 67.5; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{16}\text{H}_{14}\text{N}_4\text{O}_3\text{Na}$ 333.0964; Found 333.0960.

***trans*-3-Azido-7-chloro-1-tosyl-indolin-2-ol (**3m**)**

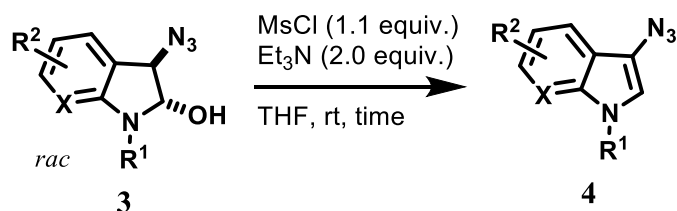


The reaction was performed according to the general procedure A using 610 mg (2.0 mmol) of **S1m**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **3m** (580 mg, 1.59 mmol, 79% yield) as a pale-yellow oil.

Pale-yellow oil (580 mg, 1.59 mmol, 79% yield); IR (KBr) ν : 3467, 3066, 2979, 2923, 2102, 1340, 1162, 758 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.75 (d, J = 8.4 Hz, 1.4H), 7.72 (d, J = 8.4 Hz, 0.6H), 7.39 (dd, J = 8.4, 1.8 Hz, 0.7H), 7.37–7.36 (m, 0.3H), 7.28–7.25 (m, 2.7H), 7.22–7.18 (m, 0.6H), 7.14 (t, J = 7.8 Hz, 0.7H), 6.06 (t, J = 4.2 Hz, 0.3H), 5.94 (d, J = 1.8 Hz, 0.7H), 4.51 (s, 0.7H), 4.38 (d, J = 4.2 Hz, 0.3H), 3.80 (d, J = 3.6 Hz, 0.7H), 3.68 (d, J = 4.2 Hz, 0.3H), 2.42 (s, 0.9H), 2.40 (s, 2.1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 144.8, 144.5, 139.1, 137.9, 136.6, 136.5, 134.4, 133.4, 132.1, 131.6, 130.0, 129.7, 127.9, 127.4, 127.2, 126.8, 126.5, 124.8, 124.4, 123.2, 92.2, 89.8, 65.7, 63.7, 21.8, 21.7; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{15}\text{H}_{13}\text{ClN}_4\text{O}_3\text{SNa}$ 387.0290, 389.0260; Found 387.0290, 389.0264.

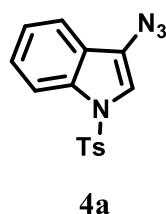
Synthesis of 3-azido-indoles **4**

General procedure B



To a solution of *trans*-3-azido-2-hydroxyindolines (AZIHYS) **3** (1.0 mmol) in THF (5 mL, 0.2 M) was added dropwise Et₃N (280 μ L, 2.0 equiv., 2.0 mmol) and MsCl (85 μ L, 1.1 equiv., 1.1 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material indicated by TLC. After the whole was quenched with H₂O (10 mL) and extracted with AcOEt (3 $\times$ 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography to give **4**.

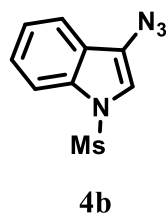
3-Azido-1-tosyl-1*H*-indole (**4a**)



The reaction was performed according to general procedure B using 165 mg (0.5 mmol) of **3a**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4a** (140 mg, 0.45 mmol, 90% yield) as a pale-yellow solid.

Pale-yellow solid (140 mg, 0.90 mmol, 90% yield; mp 83–85 °C); IR (KBr) ν : 3064, 2952, 2923, 2127, 1361, 1172, 750 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 8.00 (d, J = 7.8 Hz, 1H), 7.75 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 7.8 Hz, 1H), 7.369 (td, J = 7.8, 1.2 Hz, 1H), 7.366 (s, 1H), 7.26 (dd, J = 7.8, 1.2 Hz, 1H), 7.23 (d, J = 7.8 Hz, 2H), 2.35 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 145.4, 134.8, 134.5, 130.1, 127.0, 126.0, 125.3, 123.7, 123.4, 118.7, 114.4, 114.2, 21.7; HRMS (ESI) m/z : [M+Na]⁺ Calcd for C₁₅H₁₂N₄O₂SNa 335.0573; Found 335.0576.

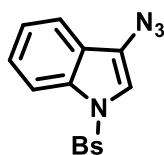
3-Azido-1-(methylsulfonyl)-1*H*-indole (**4b**)



The reaction was performed according to the general procedure B using 254 mg (1.0 mmol) of **3b**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4b** (194 mg, 0.82 mmol, 82% yield) as a pale-yellow solid.

Pale-yellow solid (194 mg, 0.82 mmol, 82% yield; mp 78–80 °C); IR (KBr) ν : 3095, 3010, 2929, 2115, 1359, 1172, 744 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.91 (d, J = 8.4 Hz, 1H), 7.64 (d, J = 7.8 Hz, 1H), 7.43 (td, J = 7.8, 1.2 Hz, 1H), 7.34 (td, J = 7.8, 0.6 Hz, 1H), 7.27 (s, 1H), 3.07 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 134.6, 126.4, 125.2, 124.0, 123.5, 119.0, 114.2, 113.6, 40.5; HRMS (ESI) m/z : $[\text{M}-\text{H}]^-$ Calcd for $\text{C}_9\text{H}_7\text{N}_4\text{O}_2\text{S}$ 235.0295; Found 235.0289.

3-Azido-1-(phenylsulfonyl)-1H-indole (**4c**)

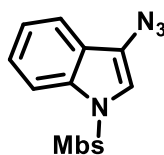


4c

The reaction was performed according to the general procedure B using 316 mg (1.0 mmol) of **3c**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4c** (274 mg, 0.92 mmol, 92% yield) as a pale-yellow solid.

Pale-yellow solid (274 mg, 0.92 mmol, 92% yield; mp 106–108 °C); IR (KBr) ν : 3112, 3052, 2111, 1371, 1174, 773 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.02 (d, J = 8.4 Hz, 1H), 7.87 (d, J = 8.4 Hz, 2H), 7.57–7.53 (m, 2H), 7.45 (t, J = 8.4 Hz, 2H), 7.380 (td, J = 7.8, 1.2 Hz, 1H), 7.375 (s, 1H), 7.26 (td, J = 7.8, 0.6 Hz, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 137.8, 134.6, 134.2, 129.5, 126.9, 126.1, 125.3, 123.8, 123.6, 118.8, 114.3, 114.2; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{14}\text{H}_{10}\text{N}_4\text{O}_2\text{SNa}$ 321.0417; Found 321.0420.

3-Azido-1-((4-methoxyphenyl)sulfonyl)-1H-indole (**4d**)



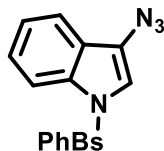
4d

The reaction was performed according to the general procedure B using 346 mg (1.0 mmol) of **3d**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4d** (297 mg, 0.90 mmol, 90% yield) as a pale-brown solid.

Pale brown solid (297 mg, 0.90 mmol, 90% yield; mp 105–107 °C); IR (KBr) ν : 3025, 2971, 2942, 2127, 1596, 1357, 1267, 1186, 1091, 759 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.00 (d, J = 9.0 Hz, 1H), 7.81 (d, J = 9.0 Hz, 2H), 7.53 (d, J = 8.4 Hz, 1H), 7.37 (td, J = 8.4, 1.2 Hz, 1H), 7.36 (s, 1H), 7.25 (td, J = 7.8, 0.6 Hz, 1H), 6.89 (d, J = 9.0 Hz, 2H), 3.80 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 164.1, 134.5, 129.26, 129.26, 126.0, 125.3,

123.7, 123.3, 118.7, 114.7, 114.4, 114.2, 55.8; HRMS (ESI) m/z : $[M+Na]^+$ Calcd for $C_{15}H_{12}N_4O_3SNa$ 351.0522; Found 351.0529.

1-([1,1'-Biphenyl]-4-ylsulfonyl)-3-azido-1*H*-indole (4e)

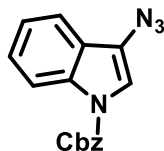


4e

The reaction was performed according to the general procedure B using 392 mg (1.0 mmol) of **3e**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4e** (276 mg, 0.74 mmol, 74% yield) as a brown solid.

Brown solid (276 mg, 0.74 mmol, 74% yield; mp 93–95 °C); IR (KBr) ν : 3100, 3068, 3025, 2121, 1369, 1172, 740 cm^{-1} ; 1H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, J = 7.8 Hz, 1H), 7.93 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 9.0 Hz, 2H), 7.56 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 9.0 Hz, 2H), 7.44 (t, J = 7.2 Hz, 2H), 7.43–7.40 (m, 2H), 7.42 (s, 1H), 7.28 (td, J = 7.8, 1.2 Hz, 1H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 147.1, 138.8, 136.1, 134.5, 129.2, 128.9, 128.0, 127.44, 127.38, 126.1, 125.3, 123.8, 123.6, 118.8, 114.3, 114.2; HRMS (ESI) m/z : $[M+H]^+$ Calcd for $C_{20}H_{15}N_4O_2S$ 375.0910; Found 375.0912.

Benzyl 3-azido-1*H*-indole-1-carboxylate (4f)

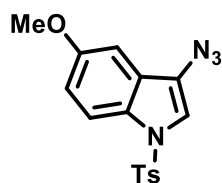


4f

The reaction was performed according to the general procedure B using 310 mg (1.0 mmol) of **3f**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4f** (263 mg, 0.90 mmol, 90% yield) as a pale-orange solid.

Pale-orange solid (263 mg, 0.90 mmol, 90% yield; mp 68–70 °C); IR (KBr) ν : 3100, 3031, 2964, 2142, 1731, 1459, 746 cm^{-1} ; 1H NMR (600 MHz, $DMSO-d_6$) δ 8.11 (d, J = 8.4 Hz, 1H), 7.75 (s, 1H), 7.58 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 7.8 Hz, 2H), 7.44–7.37 (m, 4H), 7.31 (t, J = 7.8 Hz, 1H), 5.48 (s, 2H); $^{13}C\{^1H\}$ NMR (151 MHz, $DMSO-d_6$) δ 149.9, 135.3, 133.9, 128.7, 128.6, 128.4, 125.9, 124.1, 123.5, 121.1, 118.0, 115.1, 114.7, 68.6; HRMS (ESI) m/z : $[M+Na]^+$ Calcd for $C_{16}H_{12}N_4O_2Na$ 315.0852; Found 315.0849.

3-Azido-5-methoxy-1-tosyl-1*H*-indole (4g)

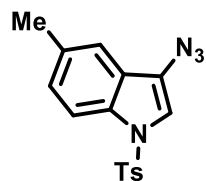


4g

The reaction was performed according to the general procedure B using 360 mg (1.0 mmol) of **3g**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4** (338 mg, 0.99 mmol, 99% yield) as a pale-brown solid.

Pale-brown solid (338 mg, 0.99 mmol, 99% yield; mp 115 °C); IR (KBr) ν : 3014, 2967, 2111, 1484, 1278, 1172, 1031, 759 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.89 (d, J = 9.0 Hz, 1H), 7.72 (d, J = 9.0 Hz, 2H), 7.33 (s, 1H), 7.22 (d, J = 7.8 Hz, 2H), 6.97 (dd, J = 9.0, 2.4 Hz, 1H), 6.90 (d, J = 2.4 Hz, 1H), 3.80 (s, 3H), 2.34 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 156.7, 145.3, 134.7, 130.0, 129.2, 126.9, 126.2, 123.6, 115.5, 115.3, 115.0, 100.6, 55.8, 21.7; HRMS (ESI) m/z : $[\text{M-H}]^-$ Calcd for $\text{C}_{16}\text{H}_{13}\text{N}_4\text{O}_3\text{S}$ 341.0714; Found 341.0713.

3-Azido-5-methyl-1-tosyl-1H-indole (**4h**)

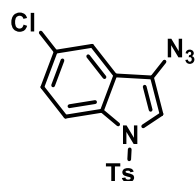


4h

The reaction was performed according to the general procedure B using 344 mg (1.0 mmol) of **3h**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4h** (320 mg, 0.98 mmol, 98% yield) as a white solid.

White solid (320 mg, 0.98 mmol, 98% yield; mp 104–106 °C); IR (KBr) ν : 2917, 2857, 2115, 1369, 1174, 761 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.88 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 8.4 Hz, 2H), 7.31 (s, 1H), 7.30 (d, J = 1.2 Hz, 1H), 7.22 (d, J = 7.8 Hz, 2H), 7.18 (dd, J = 9.0, 1.8 Hz, 1H), 2.40 (s, 3H), 2.34 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 145.2, 134.8, 133.6, 132.9, 130.0, 127.5, 126.9, 125.5, 123.2, 118.4, 114.5, 113.9, 21.7, 21.4; HRMS (ESI) m/z : $[\text{M-H}]^-$ Calcd for $\text{C}_{16}\text{H}_{13}\text{N}_4\text{O}_2\text{S}$ 325.0765; Found 325.0753.

3-Azido-5-chloro-1-tosyl-1H-indole (**4i**)

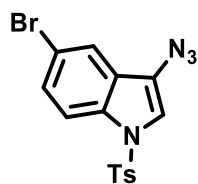


4i

The reaction was performed according to the general procedure B using 365 mg (1.0 mmol) of **3i**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4i** (322 mg, 0.93 mmol, 93% yield) as an orange solid.

Orange solid (322 mg, 0.93 mmol, 93% yield; mp 116 °C); IR (KBr) ν : 2923, 2130, 1373, 1174, 732 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.92 (d, J = 9.0 Hz, 1H), 7.73 (d, J = 9.0 Hz, 2H), 7.47 (d, J = 2.4 Hz, 1H), 7.38 (s, 1H), 7.31 (dd, J = 9.6, 2.4 Hz, 1H), 7.24 (d, J = 9.6 Hz, 2H), 2.36 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 145.7, 134.5, 132.8, 130.2, 129.7, 126.9, 126.35, 126.30, 123.0, 118.5, 115.6, 115.3, 21.8; HRMS (ESI) m/z : $[\text{M}-\text{H}]^-$ Calcd for $\text{C}_{15}\text{H}_{10}\text{ClN}_4\text{O}_2\text{S}$ 345.0218, 347.0188; Found 345.0213, 347.0183.

3-Azido-5-bromo-1-tosyl-1H-indole (**4j**)

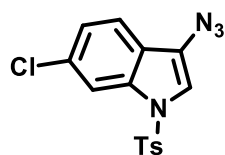


4j

The reaction was performed according to the general procedure B using 409 mg (1.0 mmol) of **3j**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4j** (387 mg, 0.99 mmol, 99% yield) as a brown solid.

Brown solid (387 mg, 0.99 mmol, 99% yield; mp 118–119 °C); IR (KBr) ν : 3093, 2923, 2125, 1375, 1172, 757 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.87 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 1.2 Hz, 1H), 7.44 (dd, J = 9.0, 2.4 Hz, 1H), 7.37 (s, 1H), 7.47 (d, J = 8.4 Hz, 2H), 2.35 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 145.7, 134.5, 133.2, 130.2, 129.0, 126.9, 126.7, 122.9, 121.5, 117.2, 115.6, 115.4, 21.7; HRMS (ESI) m/z : $[\text{M}-\text{H}]^-$ Calcd for $\text{C}_{15}\text{H}_{10}\text{N}_4\text{O}_2\text{S}$ 388.9713, 390.9692; Found 388.9707, 390.9687.

3-Azido-6-chloro-1-tosyl-1H-indole (**4k**)



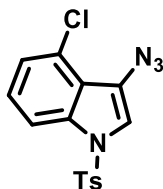
4k

The reaction was performed according to the general procedure B using 365 mg (1.0 mmol) of **3k**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4k** (346 mg, 1.00 mmol, quant.) as a pale-yellow solid.

Pale-yellow solid (346 mg, 1.00 mmol, quant.; mp 117–120 °C); IR (KBr) ν : 3095, 2927, 2113, 1363, 1172, 765 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.02 (d, J = 1.8 Hz, 1H), 7.76 (d, J = 9.0 Hz, 2H), 7.42 (d, J = 8.4 Hz, 1H), 7.35 (s, 1H), 7.27 (d, J = 9.0 Hz, 2H), 7.22 (dd, J = 9.0, 1.8 Hz, 1H), 2.37 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz,

CDCl₃) δ 145.7, 134.8, 134.6, 132.2, 130.3, 127.0, 124.5, 123.7, 123.4, 119.6, 114.7, 114.3, 21.8; HRMS (ESI) m/z : [M-H]⁻ Calcd for C₁₅H₁₀ClN₄O₂S 345.0218, 347.0188; Found 345.0220, 347.0187.

3-Azido-4-chloro-1-tosyl-1H-indole (4l)

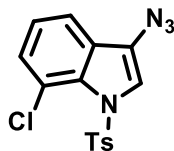


4l

The reaction was performed according to the general procedure B using 365 mg (1.0 mmol) of **3l**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4l** (350 mg, 0.98 mmol, 98% yield) as a pale-yellow solid.

Pale yellow solid (350 mg, 0.98 mmol, 98% yield; mp 105–107 °C); IR (KBr) ν : 3093, 2927, 2121, 1594, 1373, 1174, 738 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 7.91 (dd, J = 8.4, 1.2 Hz, 1H), 7.75 (d, J = 8.4 Hz, 2H), 7.48 (s, 1H), 7.27–7.24 (m, 3H), 7.20 (dd, J = 8.4, 1.2 Hz, 1H), 2.37 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 145.8, 135.7, 134.4, 130.2, 127.0, 126.5, 126.0, 125.0, 123.8, 122.1, 116.0, 112.6, 21.8; HRMS (ESI) m/z : [M-H]⁻ Calcd for C₁₅H₁₀ClN₄O₂S 345.0218, 347.0188; Found 345.0215, 347.0195.

3-Azido-7-chloro-1-tosyl-1H-indole (4m)

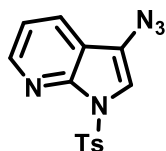


4m

The reaction was performed according to the general procedure B using 365 mg (1.0 mmol) of **3m**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4m** (310 mg, 0.89 mmol, 89% yield) as a pale-yellow solid.

Pale-yellow solid (310 mg, 0.89 mmol, 89% yield; mp 107–109 °C); IR (KBr) ν : 3066, 2923, 2127, 1365, 1172, 781 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 7.76 (s, 1H), 7.72 (d, J = 8.4 Hz, 2H), 7.45 (dd, J = 7.8, 0.6 Hz, 1H), 7.28 (d, J = 7.8 Hz, 2H), 7.27 (d, J = 7.2 Hz, 1H), 7.15 (t, J = 7.8 Hz, 1H), 2.40 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 145.2, 136.7, 131.4, 129.9, 128.9, 128.2, 127.4, 124.5, 122.0, 119.6, 118.6, 117.4, 21.8; HRMS (ESI) m/z : [M+Na]⁺ Calcd for C₁₅H₁₀ClN₄O₂S 345.0218, 347.0188; Found 345.0217, 347.0191.

3-Azido-1-tosyl-1H-pyrrolo[2,3-*b*]pyridine (4n)

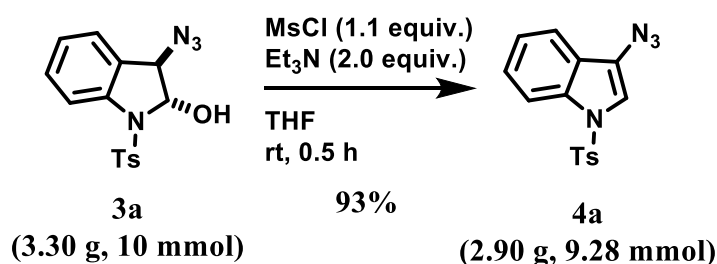


4n

The reaction was performed according to the general procedure B using 331 mg (1.0 mmol) of **3n**. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **4n** (273 mg, 0.87 mmol, 87% yield) as a white solid.

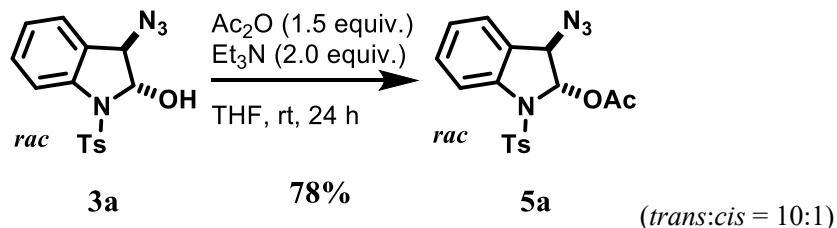
White solid (273 mg, 0.87 mmol, 87% yield; mp 110–112 °C); IR (KBr) ν : 3087, 2925, 2111, 1594, 1361, 1172, 763 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.48 (dd, $J = 4.2, 1.8$ Hz, 1H), 8.05 (d, $J = 8.4$ Hz, 2H), 7.86 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.54 (s, 1H), 7.28 (d, $J = 8.4$ Hz, 2H), 7.20 (dd, $J = 7.8, 4.2$ Hz, 1H), 2.37 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 146.3, 146.0, 145.6, 135.2, 129.9, 128.2, 127.4, 119.9, 119.1, 117.7, 114.5, 21.8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{14}\text{H}_{11}\text{N}_5\text{O}_2\text{SNa}$ 336.0526; Found 336.0530.

Gram scale synthesis of 3-azidoindole (AZIND)



To a solution of **3a** (3.30 g, 10 mmol) and Et_3N (2.77 mL, 2.0 equiv., 20 mmol) in THF (50 mL, 0.2 M) was added MsCl (0.851 mL, 1.1 equiv., 11 mmol). The mixture was stirred at room temperature for 0.5 h. After the addition of H_2O (50 mL), the whole was extracted with AcOEt (3×50 mL). The combined organic layer was washed with brine (50 mL), dried over Na_2SO_4 , and concentrated *in vacuo*. The residue was purified by recrystallization using MeOH to give **4a** as a pale-yellow solid (2.90 g, 9.28 mmol, 93% yield).

trans-3-Azido-1-tosylindolin-2-yl acetate (**5a**)



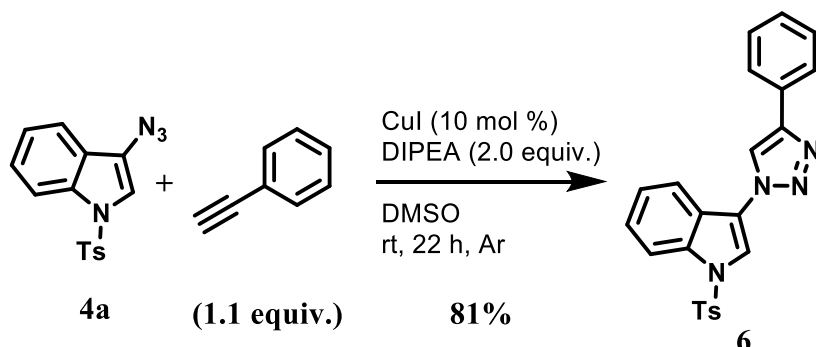
To a solution of *trans*-3-Azido-2-hydroxy-1-tosylindoline **3a** (165 mg, 0.5 mmol) in THF (2.5 mL, 0.2 M) was added dropwise Et_3N (140 μL , 2.0 equiv., 1.0 mmol) and MsCl (60 μL , 1.5 equiv., 0.75 mmol) under air. The mixture was stirred at room temperature for 24 h. After the whole was quenched with H_2O (10 mL) and extracted with AcOEt (3×20 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 (4/1–3/1 [v/v]) to give **5a** (145 mg, 0.39 mmol, 78% yield) as an orange oil.

Orange oil (145 mg, 0.39 mmol, 78% yield); IR (KBr) ν : 2927, 2103, 1749, 1363, 1222, 1172, 1016, 756 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.73 (d, J = 7.8 Hz, 2H), 7.67 (d, J = 8.4 Hz, 1H), 7.41 (td, J = 8.4 1.2 Hz, 1H), 7.30 (d, J = 7.2 Hz, 1H), 7.25 (d, J = 8.4 Hz, 2H), 7.15 (dt, J = 7.8, 0.6 Hz, 1H), 6.51 (s, 1H), 4.56 (s, 1H), 2.36 (s, 3H), 2.08 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 169.6, 145.1, 141.6, 134.9, 131.3, 130.1, 127.2, 126.1, 125.9, 124.8, 115.5, 89.8, 65.6, 21.7, 21.0; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{17}\text{H}_{16}\text{N}_4\text{O}_4\text{SNa}$ 395.0784; Found 395.0783.

Transformation of 3-azidoindole

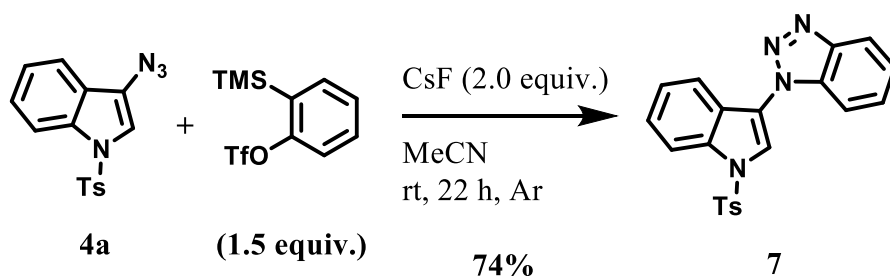
3-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)-1-tosyl-1*H*-indole (**6**)



To a mixture of 3-Azido-1-tosyl-1*H*-indole **4a** (62.5 mg, 0.20 mmol) and CuI (3.8 mg, 10 mol%, 0.02 mmol) in DMSO (1 mL, 0.2 M) was added dropwise DIPEA (68 μ L, 2.0 equiv., 0.40 mmol) and Ethynylbenzene (24 μ L, 1.1 equiv., 0.22 mmol) under argon. The mixture was stirred at room temperature for 22 h. After the whole was quenched with H₂O (10 mL) and filtrated through celite pa with AcOEt (30 mL). The filtrate was extracted with AcOEt (3 $\times$ 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography using hexane/AcOEt (2/1–1/1 [v/v]) to give **6** (66.9 mg, 0.161 mmol, 81% yield) as a Pale-purple solid.

Pale-purple solid (66.9 mg, 0.161 mmol, 81% yield; mp 180–182 °C); IR (KBr) ν : 3031, 1438, 1367, 1172, 761 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 8.21 (s, 1H), 8.08 (d, J = 8.4 Hz, 1H), 8.00 (s, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.92 (d, J = 7.8 Hz, 2H), 7.84 (d, J = 9.0 Hz, 2H), 7.48–7.44 (m, 3H), 7.39–7.35 (m, 2H), 7.25 (d, J = 7.8 Hz, 2H), 2.35 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 148.0, 145.9, 134.6, 134.2, 130.3, 130.0, 129.1, 128.7, 127.2, 126.5, 126.0, 124.6, 123.8, 121.4, 120.4, 129.3, 117.6, 113.9, 21.7; HRMS (ESI) m/z : [M+Na]⁺ Calcd for C₂₃H₁₈N₄O₂SNa 437.1043; Found 437.1047.

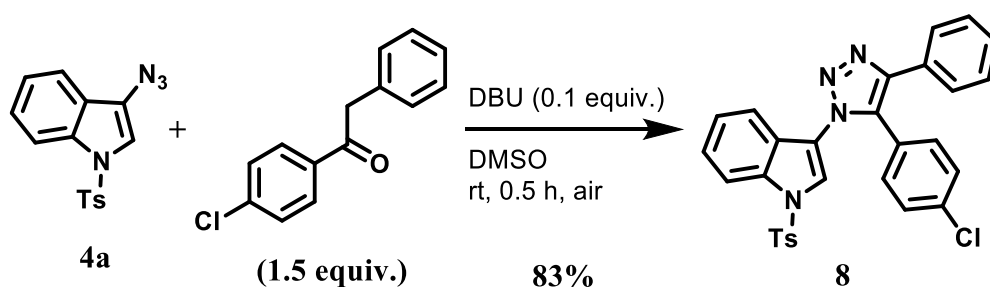
1-(1-Tosyl-1*H*-indol-3-yl)-1*H*-benzo[d][1,2,3]triazole (**7**)



To a solution of 3-Azido-1-tosyl-1*H*-indole **4a** (62.5 mg, 0.20 mmol) and 2-(Trimethylsilyl)phenyl Trifluoromethanesulfonate (89.5 mg, 1.5 equiv., 0.30 mmol) in MeCN (1 mL, 0.2 M) was added CsF (60.8 mg, 2.0 equiv., 0.40 mmol) under Ar. The mixture was stirred at room temperature for 22 h. After the whole was quenched with H₂O (10 mL) and extracted with AcOEt (3 $\times$ 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography using hexane/AcOEt (2/1–1/1 [v/v]) to give **7** (57.5 mg, 0.148 mmol, 74% yield) as a pale-yellow solid.

Pale-yellow solid (57.5 mg, 0.148 mmol, 74% yield; mp 113–115 °C); IR (KBr) ν : 3073, 3031, 1444, 1371, 1174, 740 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.18 (d, J = 8.4 Hz, 1H), 8.13 (d, J = 9.0 Hz, 1H), 8.04 (s, 1H), 7.87 (d, J = 7.8 Hz, 2H), 7.79 (d, J = 7.8 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.59 (td, J = 8.4, 1.2 Hz, 1H), 7.49–7.46 (m, 2H), 7.34 (td, J = 7.2, 0.6 Hz, 1H), 7.28 (d, J = 7.8 Hz, 2H), 2.36 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 146.0, 145.9, 134.7, 134.2, 133.2, 130.3, 128.7, 127.2, 126.5, 125.0, 124.8, 124.5, 120.54, 120.52, 120.47, 118.7, 114.0, 110.4, 21.8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{21}\text{H}_{16}\text{N}_4\text{O}_2\text{SNa}$ 411.0886; Found 411.0892.

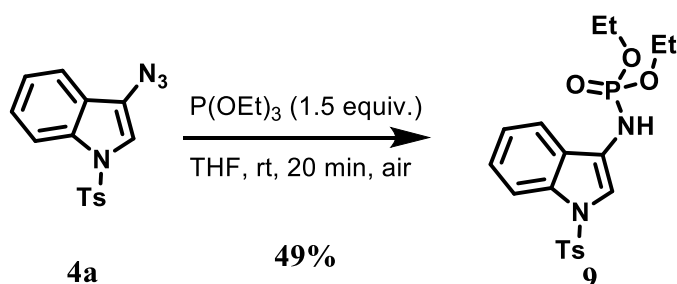
3-(5-(4-Chlorophenyl)-4-phenyl-1H-1,2,3-triazol-1-yl)-1-tosyl-1H-indole (8)



To a solution of 3-Azido-1-tosyl-1H-indole **4a** (62.5 mg, 0.20 mmol) and Benzyl 4-Chlorophenyl Ketone (69.2 mg, 1.5 equiv., 0.30 mmol) in DMSO (1 mL, 0.2 M) was added dropwise DBU (3 μL , 0.1 equiv., 0.02 mmol) under air. The mixture was stirred at room temperature for 0.5 h. After the whole was quenched with H_2O (10 mL) and extracted with AcOEt (3×20 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 (2/1–1/1 [v/v]) to give **8** (87.3 mg, 0.166 mmol, 83% yield) as a pale-yellow solid.

Pale-yellow solid (87.3 mg, 0.166 mmol, 83% yield; mp 165–166 °C); IR (KBr) ν : 3056, 2921, 1596, 1378, 1176, 748 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.03 (d, J = 9.0 Hz, 1H), 7.63–7.59 (m, 5H), 7.42 (td, J = 7.8, 1.2 Hz, 1H), 7.37–7.29 (m, 7H), 7.27 (d, J = 9.0 Hz, 2H), 7.16 (d, J = 8.4 Hz, 2H), 2.40 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 145.9, 144.6, 136.0, 124.5, 133.7, 133.4, 131.4, 130.25, 130.25, 129.7, 128.8, 128.4, 127.4, 127.1, 126.4, 125.9, 125.7, 124.6, 121.0, 120.0, 119.5, 113.8, 21.8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{29}\text{H}_{21}\text{N}_4\text{O}_2\text{SNa}$ 548.0966, 549.0937; Found 548.0968, 549.0942.

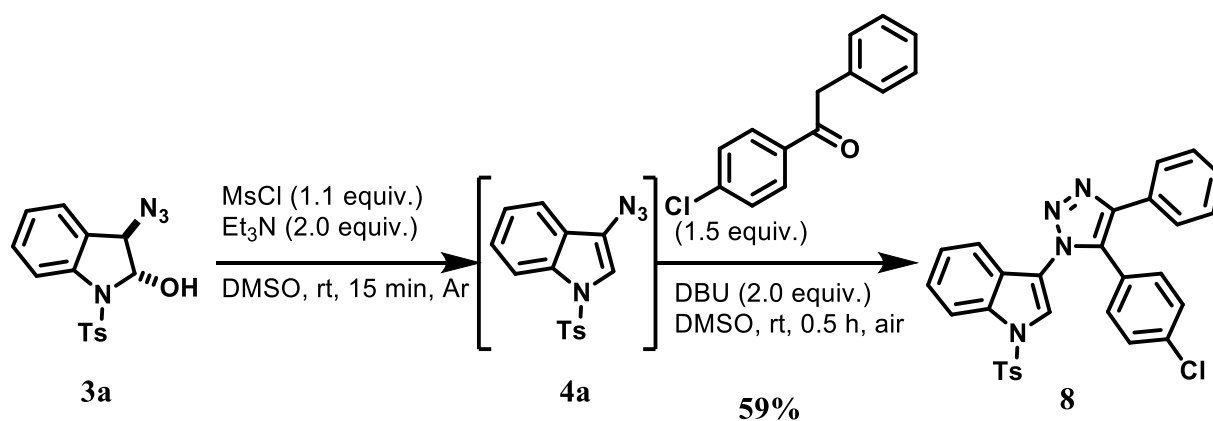
Diethyl (1-tosyl-1H-indol-3-yl)phosphoramidate (9)



To a solution of 3-Azido-1-tosyl-1*H*-indole **4a** (62.5 mg, 0.20 mmol) in THF (1 mL, 0.2 M) was added P(OEt)₃ (52 μ L, 1.5 equiv., 0.30 mmol) under air. The mixture was stirred at room temperature for 20 min. After the whole was quenched with H₂O (10 mL) and extracted with AcOEt (3 $\times$ 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **9** (41.4 mg, 0.10 mmol, 49% yield) as a pale-yellow oil.

Pale-yellow oil (41.4 mg, 0.10 mmol, 49% yield); IR (KBr) ν : 3166, 2985, 2950, 1365, 1241, 1174, 763 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 8.02 (d, J = 7.8 Hz, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.69 (d, J = 8.4 Hz, 2H), 7.34 (td, J = 7.8, 0.6 Hz, 1H), 7.25 (td, J = 7.8, 0.6 Hz, 1H), 7.19 (s, 1H), 7.15 (d, J = 8.4 Hz, 2H), 7.12 (d, J = 10.2 Hz, 1H), 4.17–4.13 (m, 2H), 4.05–4.01 (m, 2H), 2.31 (s, 3H), 1.28 (t, J = 7.2 Hz, 6H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 144.8, 134.9, 134.3, 129.7, 126.8, 126.1 (d, J_{C-P} = 11.6 Hz), 125.5, 123.7, 123.5, 118.6, 114.2, 111.1, 63.0 (d, J_{C-P} = 5.9 Hz), 21.6, 16.2 (d, J_{C-P} = 7.2 Hz); HRMS (ESI) m/z : [M+Na]⁺ Calcd for C₁₉H₂₃N₂O₅PSNa 445.0958; Found 445.0963.

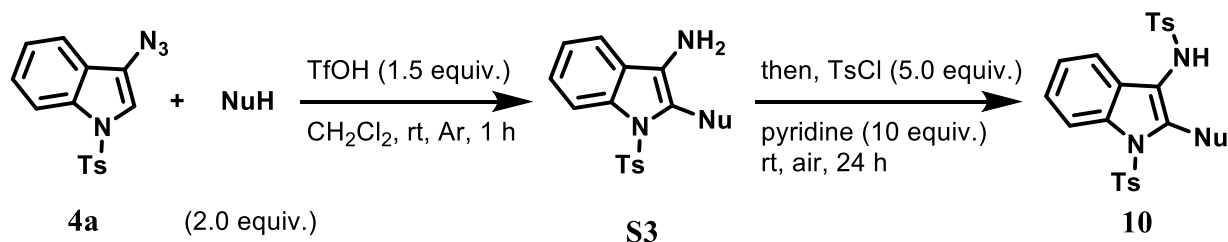
One-pot protocol for the synthesis of triazole



To the solution of *trans*-3-azido-2-hydroxyindolines (AZIHYs) **3** (66.1 mg, 0.2 mmol) in DMSO (1 mL, 0.2 M) was added dropwise Et₃N (55 μ L, 2.0 equiv., 0.4 mmol) and MsCl (17 μ L, 1.1 equiv., 0.22 mmol) under air. The mixture was stirred at room temperature for 15 min. Then, Benzyl 4-Chlorophenyl Ketone (69.2 mg, 1.5 equiv., 0.30 mmol) and DBU (66 μ L, 2.2 equiv., 0.44 mmol) was added to the mixture. After the mixture was stirred for a further 0.5 h, the whole was quenched with H₂O (10 mL) and extracted with AcOEt (3 $\times$ 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography using hexane/AcOEt (2/1–1/1 [v/v]) to give **8** (61.9 mg, 0.12 mmol, 59% yield) as a pale-yellow solid.

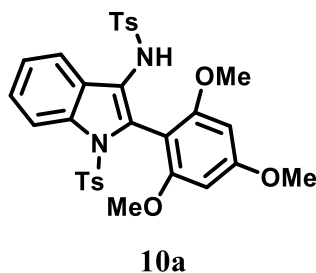
cine-Substitution of 3-azidoindoles

General procedure C



To the solution of 3-Azido-1-tosyl-*LH*-indole **4a** (62.5 mg, 0.20 mmol) and nucleophile (2 equiv.) in CH₂Cl₂ (1 mL, 0.2 M) was added dropwise TfOH (26 μ L, 1.5 equiv., 0.3 mmol) under argon. The mixture was stirred at room temperature for 1 h. Then, pyridine (160 μ L, 10 equiv., 2.0 mmol) and TsCl (190 mg, 5.0 equiv., 1.0 mmol) were added to the mixture under air. After the mixture was stirred for a further 24 h, the whole was quenched with H₂O (10 mL) and extracted with AcOEt (3 $\times$ 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography using hexane/AcOEt to give **10**.

4-Methyl-*N*-(1-tosyl-2-(2,4,6-trimethoxyphenyl)-*LH*-indol-3-yl)benzenesulfonamide (**10a**)

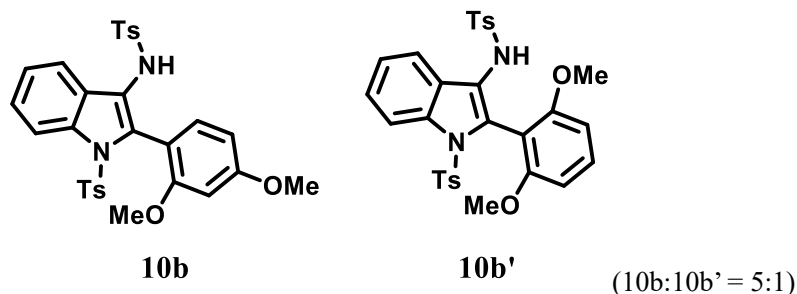


The reaction was performed according to the general procedure C using 62.5 mg (0.20 mmol) of **4a** and 67.3 mg of 1,3,5-trimethoxybenzene (0.40 mmol). The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–1/1 [v/v]) to give **10a** (114 mg, 0.19 mmol, 94% yield) as a pale-purple solid.

Pale-purple solid (114 mg, 0.19 mmol, 94% yield; mp 193–195 °C); IR (KBr) ν : 3291, 3054, 2973, 2940, 1616, 1585, 1365, 1228, 1128, 1037, 759 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 8.17 (dd, J = 7.8, 1.8 Hz, 1H), 7.94 (dd, J = 6.6, 2.4 Hz, 1H), 7.33–7.30 (m, 2H), 7.22 (d, J = 8.4 Hz, 2H), 7.20 (d, J = 8.4 Hz, 2H), 6.99 (d, J = 7.8 Hz, 2H), 6.91 (d, J = 7.8 Hz, 2H), 6.45 (s, 1H), 5.96 (s, 2H), 3.87 (s, 3H), 3.58 (s, 6H), 2.35 (s, 3H), 2.25 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 162.9, 159.0, 144.3, 142.4, 136.4, 136.0, 135.6, 129.2, 129.0, 128.3, 128.1, 127.0, 126.7, 125.1, 124.0, 120.3, 119.8, 115.4, 99.7, 90.2, 55.6, 55.5, 21.8, 21.6; HRMS (ESI) m/z : [M+Na]⁺ Calcd for C₃₁H₃₀N₂O₇S₂Na 629.1387; Found 629.1388.

N-(2-(2,4-dimethoxyphenyl)-1-tosyl-*LH*-indol-3-yl)-4-methylbenzenesulfonamide (**10b**)

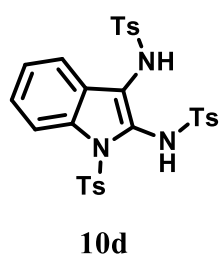
N-(2-(2,6-dimethoxyphenyl)-1-tosyl-*LH*-indol-3-yl)-4-methylbenzenesulfonamide (**10b'**)



The reaction was performed according to the general procedure C using 62.5 mg (0.20 mmol) of **4a** and 55.3 mg of 1,3-dimethoxybenzene (0.40 mmol). The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–1/1 [v/v]) to give **10b** and **10b'** (111 mg, 0.19 mmol, 96% yield) as a white solid.

White solid (111 mg, 0.19 mmol, 96% yield; mp 178–179 °C); IR (KBr) ν : 3315, 3096, 3062, 2975, 2944, 1594, 1506, 1365, 1209, 1176, 1039, 761 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.25 (d, J = 7.8 Hz, 0.8H), 8.16 (d, J = 7.2 Hz, 0.2H), 7.96 (d, J = 7.8 Hz, 0.2H), 7.93 (d, J = 8.4 Hz, 0.8H), 7.39–7.27 (m, 2.2H), 7.20 (d, J = 7.8 Hz, 0.4H), 7.17 (d, J = 7.8 Hz, 0.4H), 7.11 (d, J = 8.4 Hz, 1.6H), 7.08 (d, J = 8.4 Hz, 1.6H), 7.00 (d, J = 7.8 Hz, 0.4H), 6.98 (d, J = 8.4 Hz, 1.6H), 6.89 (d, J = 7.8 Hz, 1.6H), 6.87 (d, J = 7.8 Hz, 0.4H), 6.51 (d, J = 9.0 Hz, 0.8H), 6.50–6.47 (m, 1H), 6.41 (d, J = 7.8 Hz, 0.4H), 6.38 (d, J = 2.4 Hz, 0.8H), 6.26 (dd, J = 8.4, 2.4 Hz, 0.8H), 3.86 (s, 2.4H), 3.68 (s, 2.4H), 3.61 (s, 1.2H), 2.341 (s, 2.4H), 2.335 (s, 0.6H), 2.27 (s, 2.4H), 2.26 (s, 0.6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 161.7, 158.4, 156.5, 144.7, 144.4, 143.2, 142.5, 136.9, 136.4, 135.7, 135.5, 135.2, 135.0, 134.6, 131.4, 131.09, 131.09, 129.3, 129.21, 129.15, 128.1, 128.0, 127.9, 126.83, 126.83, 126.82, 126.7, 125.5, 125.3, 124.6, 124.0, 120.6, 120.5, 120.4, 120.1, 116.1, 115.3, 109.9, 106.8, 104.4, 103.5, 98.0, 56.0, 55.7, 55.6, 21.8, 21.7, 21.64, 21.60; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{30}\text{H}_{28}\text{N}_2\text{O}_6\text{S}_2\text{Na}$ 599.1281; Found 599.1283.

N,N'-(1-Tosyl-1*H*-indole-2,3-diyl)bis(4-methylbenzenesulfonamide) (**10d**)

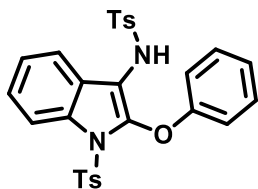


The reaction was performed according to the general procedure C using 62.5 mg (0.2 mmol) of **4a** and 68.5 mg of tosylamide (0.40 mmol). The residue was purified by silica gel column chromatography using toluene/AcOEt (20/1–10/1 [v/v]) to give **10d** (74.9 mg, 0.12 mmol, 61% yield) as a purple oil.

Purple oil (74.9 mg, 0.12 mmol, 61% yield); IR (KBr) ν : 3274, 3064, 3031, 2923, 1596, 1363, 1164, 752 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 7.91 (br s, 1H), 7.82 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.29–7.23 (m, 4H), 7.20–7.18 (m, 4H), 7.12 (d, J = 7.8 Hz, 2H), 7.07 (br s, 1H), 2.49 (s, 3H), 2.38 (s, 3H), 2.37 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 146.1., 145.4, 144.0, 136.3,

134.3, 133.7, 133.0, 130.0, 129.9, 129.5, 127.80, 127.76, 126.6, 126.54, 126.45, 125.0, 121.4, 117.8, 114.25, 114.25, 21.9, 21.85, 21.83; HRMS (ESI) m/z : $[M+Na]^+$ Calcd for $C_{29}H_{27}N_3O_6S_3Na$ 632.0954; Found 632.0956.

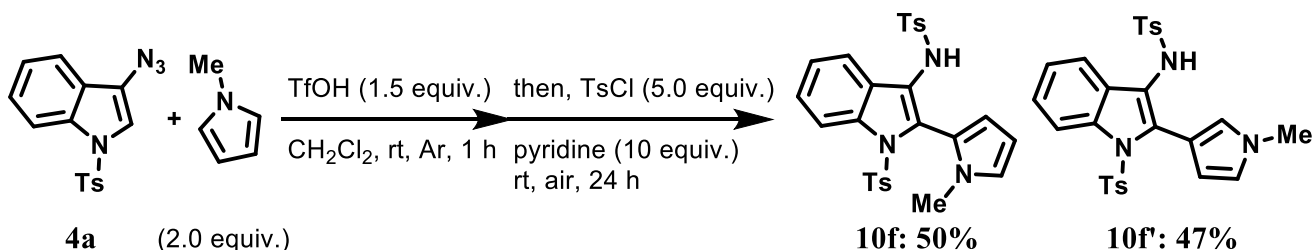
4-Methyl-*N*-(2-phenoxy-1-tosyl-1*H*-indol-3-yl)benzenesulfonamide (10e)



10e

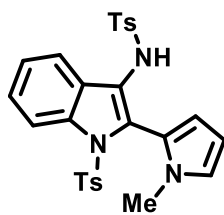
The reaction was performed according to the general procedure C using 62.5 mg (0.2 mmol) of **4a** and 37.6 mg of phenol (0.4 mmol). The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **10e** (33.7 mg, 0.063 mmol, 32% yield) as a brown oil.

Brown oil (33.7 mg, 0.063 mmol, 32% yield); IR (KBr) ν : 3261, 3064, 2923, 1596, 1375, 1160, 1086, 754 cm^{-1} ; 1H NMR (600 MHz, $CDCl_3$) δ 8.19 (d, J = 9.0 Hz, 1H), 7.62–7.63 (m, 3H), 7.37–7.34 (m, 3H), 7.30 (td, J = 7.8, 1.2 Hz, 1H), 7.19 (d, J = 8.4 Hz, 2H), 7.18 (t, J = 7.8 Hz, 2H), 7.05 (t, J = 7.2 Hz, 1H), 7.03 (d, J = 7.8 Hz, 2H), 6.56 (d, J = 8.4 Hz, 2H), 5.71 (s, 1H), 2.41 (s, 3H), 2.40 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 157.2, 145.5, 143.8, 141.1, 136.0, 135.2, 130.8, 129.86, 129.86, 129.5, 127.4, 127.2, 125.8, 125.3, 124.5, 123.7, 119.6, 115.2, 114.5, 105.1, 21.84, 21.80; HRMS (ESI) m/z : $[M+Na]^+$ Calcd for $C_{28}H_{24}N_2O_5S_2Na$ 555.1019; Found 555.1024.



The reaction was performed according to the general procedure C using 62.5 mg (0.2 mmol) of **4a** and 32.4 mg of 1-methylpyrrole (0.4 mmol). The residue was purified by silica gel column chromatography using hexane/AcOEt (4/1–2/1 [v/v]) to give **10f** (52.4 mg, 0.100 mmol, 50% yield, pale-gray oil) and **10f'** (48.6 mg, 0.094 mmol, 47% yield pale-purple solid).

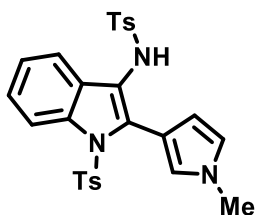
4-Methyl-*N*-(2-(1-methyl-1*H*-pyrrol-2-yl)-1-tosyl-1*H*-indol-3-yl)benzenesulfonamide (10f)



10f

Pale-gray oil (52.4 mg, 0.100 mmol, 50% yield); IR (KBr) ν : 3253, 3050, 3031, 2946, 1596, 1357, 1170, 754 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.27 (d, J = 7.8 Hz, 1H), 7.73 (d, J = 7.2 Hz, 1H), 7.34 (td, J = 7.8, 1.8 Hz, 1H), 7.29 (d, J = 8.4 Hz, 2H), 7.27 (t, J = 7.8 Hz, 1H), 7.25 (d, J = 8.4 Hz, 2H), 7.08–7.06 (m, 4H), 6.49 (t, J = 2.4 Hz, 1H), 6.12 (br s, 1H), 5.85 (t, J = 1.8 Hz, 1H), 5.61 (dd, J = 3.0, 1.8 Hz, 1H), 3.57 (s, 3H), 2.42 (s, 3H), 2.34 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 144.6, 143.6, 135.9, 135.4, 135.2, 130.8, 129.31, 129.31, 129.29, 127.6, 127.1, 125.2, 124.2, 123.7, 121.6, 120.3, 118.7, 115.7, 111.3, 109.5, 36.4, 21.72, 21.72; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{27}\text{H}_{25}\text{N}_3\text{O}_4\text{S}_2\text{Na}$ 542.1179; Found 542.1183.

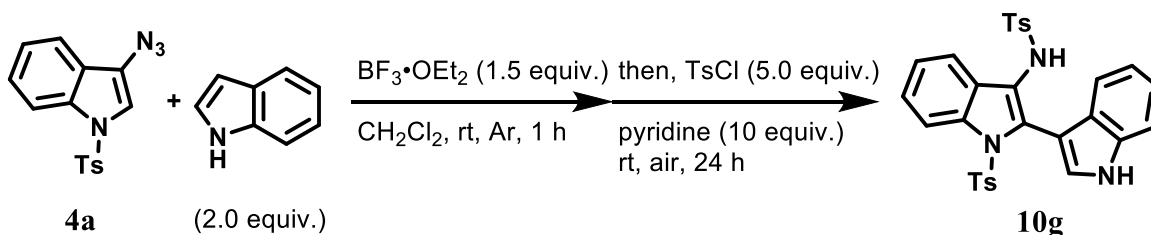
4-Methyl-N-(2-(1-methyl-1H-pyrrol-3-yl)-1-tosyl-1H-indol-3-yl)benzenesulfonamide (10f')



10f'

Pale-purple solid (48.6 mg, 0.094 mmol, 47% yield; mp 171–172 $^{\circ}\text{C}$); IR (KBr) ν : 3284, 3052, 2979, 2948, 2923, 1594, 1373, 1178, 755 cm^{-1} ; ^1H NMR (600 MHz, CDCl_3) δ 8.28 (d, J = 7.8 Hz, 1H), 8.03 (d, J = 7.8 Hz, 1H), 7.43 (t, J = 8.4 Hz, 1H), 7.36 (td, J = 7.8, 1.2 Hz, 1H), 7.34 (d, J = 9.0 Hz, 2H), 7.21 (d, J = 8.4 Hz, 2H), 7.09–7.07 (m, 4H), 6.69 (t, J = 2.4 Hz, 1H), 6.59 (br s, 1H), 6.14 (dd, J = 4.2, 3.0 Hz, 1H), 5.56 (dd, J = 3.6, 1.2 Hz, 1H), 2.96 (s, 3H), 2.40 (s, 3H), 2.33 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 145.2, 143.7, 136.0, 135.1, 134.3, 129.5, 129.4, 127.4, 127.1, 126.7, 126.3, 125.2, 124.9, 124.6, 122.0, 121.6, 119.2, 115.5, 112.2, 108.0, 34.5, 21.73, 21.67; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ Calcd for $\text{C}_{27}\text{H}_{25}\text{N}_3\text{O}_4\text{S}_2\text{Na}$ 542.1179; Found 542.1183.

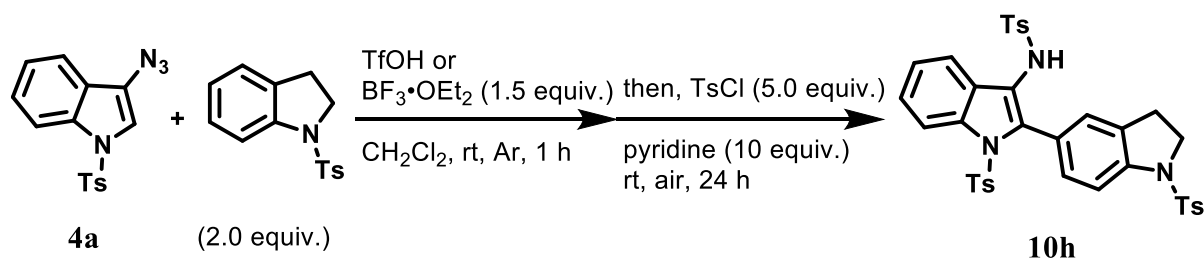
4-Methyl-N-(1-tosyl-1H,1'H-[2,3'-biindol]-3-yl)benzenesulfonamide (10g)



To the solution of 3-Azido-1-tosyl-1H-indole **4a** (62.5 mg, 0.20 mmol) and indole (46.9 mg, 2.0 equiv., 0.4 mmol) in CH_2Cl_2 (1 mL, 0.2 M) was added dropwise $\text{BF}_3 \cdot \text{OEt}_2$ (38 μL , 1.5 equiv., 0.3 mmol) under argon. The mixture was

stirred at room temperature for 1 h. Then, pyridine (160 μ L, 10 equiv., 2.0 mmol) and TsCl (190 mg, 5.0 equiv., 1.0 mmol) was added to the mixture under air. After the mixture was stirred for a further 24 h, the whole was quenched with H₂O (10 mL) and extracted with AcOEt (3 $\times$ 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography using toluene/AcOEt (20/1–10/1 [v/v]) to **10g** (80.5 mg, 0.15 mmol, 73% yield) as a brown oil. Brown oil (80.5 mg, 0.15 mmol, 73% yield); IR (KBr) ν : 3369, 3054, 3031, 2921, 1596, 1373, 1164, 754 cm^{-1} ; ¹H NMR (600 MHz, CDCl₃) δ 8.36 (d, J = 8.4 Hz, 1H), 8.31 (br s, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.42 (ddd, J = 8.4, 7.2, 1.2 Hz, 1H), 7.38 (d, J = 7.8 Hz, 1H), 7.35 (td, J = 7.8, 0.6 Hz, 1H), 7.21 (t, J = 7.2 Hz, 1H), 7.08–7.05 (m, 4H), 7.01 (t, J = 7.8 Hz, 1H), 6.94 (d, J = 7.8 Hz, 2H), 6.85 (d, J = 7.8 Hz, 2H), 6.80 (d, J = 7.8 Hz, 1H), 6.58 (d, J = 2.4 Hz, 1H), 6.05 (br s, 1H), 2.35 (s, 3H), 2.22 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 144.8, 143.6, 136.4, 135.2, 135.1, 134.5, 129.3, 129.2, 127.5, 127.05, 127.05, 126.75, 126.75, 125.5, 124.4, 122.7, 120.9, 120.3, 119.4, 118.8, 115.77, 115.77, 111.8, 103.1, 21.6, 21.5; HRMS (ESI) m/z : [M+Na]⁺ Calcd for C₃₀H₂₅N₃O₄S₂Na 587.1179; Found 587.1184.

4-Methyl-*N*-(1-tosyl-2-(1-tosylindolin-5-yl)-1*H*-indol-3-yl)benzenesulfonamide (**10h**)



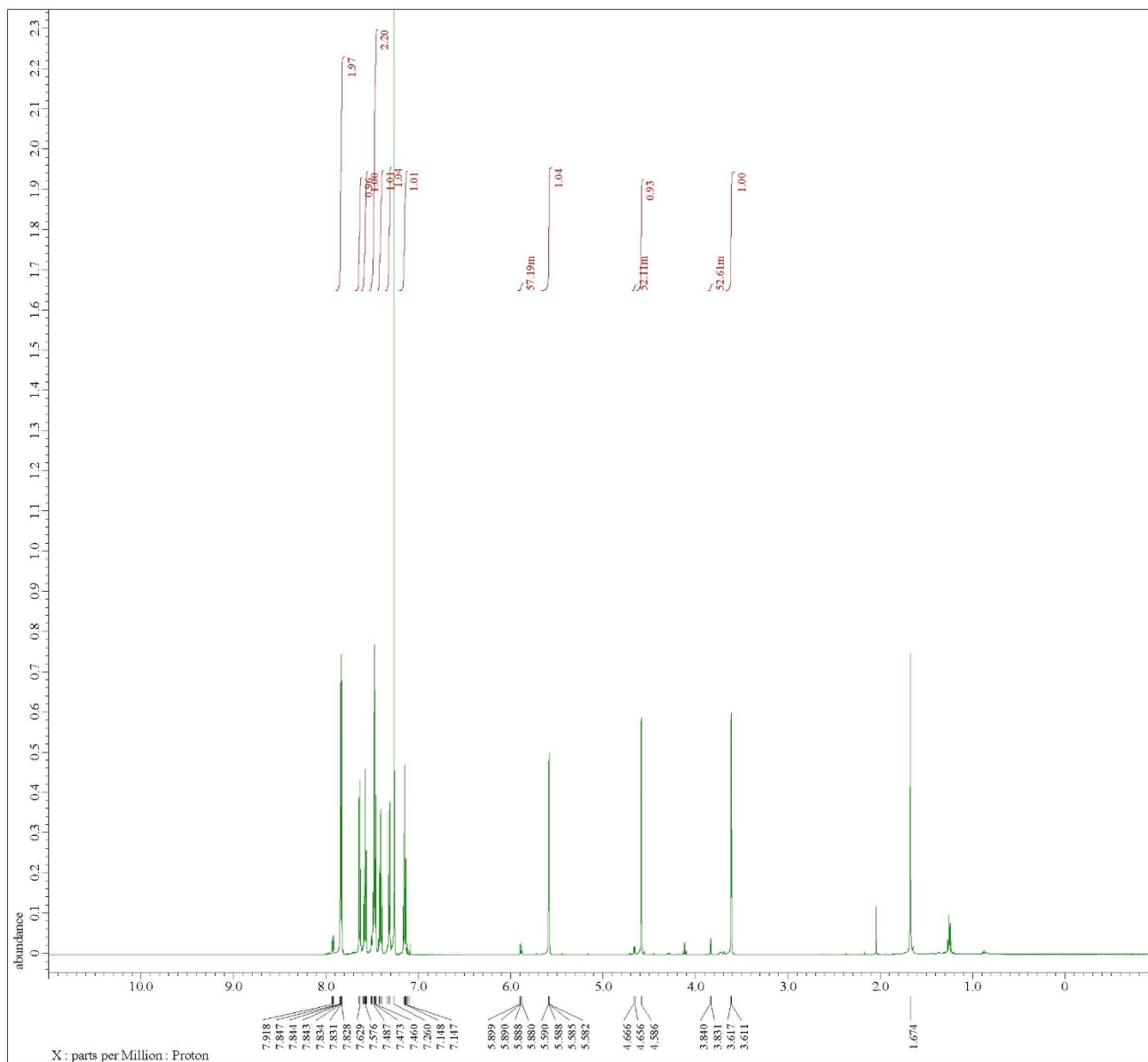
To the solution of 3-Azido-1-tosyl-1*H*-indole **4a** (62.5 mg, 0.20 mmol) and *N*-tosylindoline (109.3 mg, 2.0 equiv., 0.40 mmol) in CH₂Cl₂ (1 mL, 0.2 M) was added dropwise TfOH (26 μ L, 1.5 equiv., 0.3 mmol) or BF₃·OEt₂ (38 μ L, 1.5 equiv., 0.3 mmol) under argon. The mixture was stirred at room temperature for 1 h. Then, pyridine (160 μ L, 10 equiv., 2.0 mmol) and TsCl (190 mg, 5.0 equiv., 1.0 mmol) was added to the mixture under air. After the mixture was stirred for a further 24 h, the whole was quenched with H₂O (10 mL) and extracted with AcOEt (3 $\times$ 20 mL). The combined organic layer was washed with brine (20 mL), dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography using toluene/AcOEt (20/1–10/1 [v/v]) to give **10h** (TfOH: 69.7 mg, 0.10 mmol, 49% yield, BF₃·OEt₂: 81.9 mg, 0.12 mmol, 58% yield) as a gray oil.

Gray oil (TfOH: 69.7 mg, 0.10 mmol, 49% yield, BF₃·OEt₂: 81.9 mg, 0.12 mmol, 58% yield); IR (KBr) ν : 3291, 3064, 3064, 3029, 2954, 2921, 1596, 1355, 1172, 757 cm^{-1} ; ¹H NMR (600 MHz, CDCl₃) δ 8.29 (d, J = 9.0 Hz, 1H), 7.85 (d, J = 7.2 Hz, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 7.8 Hz, 1H), 7.41 (t, J = 7.8 Hz, 1H), 7.35–7.33 (m, 3H), 7.16 (d, J = 8.4 Hz, 2H), 7.07 (d, J = 8.4 Hz, 2H), 7.02 (d, J = 8.4 Hz, 2H), 6.86 (d, J = 7.8 Hz, 2H), 6.42 (dd, J = 8.4, 1.8 Hz, 1H), 6.32 (d, J = 0.6 Hz, 1H), 6.19 (br s, 1H), 3.95 (br s, 2H), 2.77 (br s, 2H), 2.39 (s, 3H), 2.37 (s, 3H), 2.33 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 145.2, 144.8, 143.6, 142.9, 135.9, 135.2, 135.0, 134.2, 133.9, 131.4, 130.0, 129.9, 129.5, 129.4, 128.0, 127.5, 127.4, 127.1, 126.8, 126.0, 124.6,

123.5, 120.9, 119.2, 115.6, 113.8, 50.2, 27.6, 21.8, 21.73, 21.73; HRMS (ESI) m/z : $[M+Na]^+$ Calcd for $C_{37}H_{33}N_3O_6S_3Na$ 734.1424; Found 734.1416.

Reference

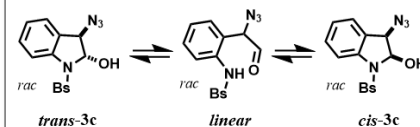
- 1) (a) Rivinoja, D. J.; Gee, Y. S.; Gardiner, M. G.; Ryan, J. H.; Hyland, C. J. T. *ACS Catal.* **2017**, *7*, 1053–1056; (b) Arisawa, M.; Terada, Y.; Takahashi, K.; Nakagawa, M.; Nishida, A. *J. Org. Chem.* **2006**, *71*, 4255–4261; (c) Yoshida, K.; Hayashi, K.; Yanagisawa, A. *Org. Lett.* **2011**, *13*, 4762–4765; (d) Liu, Q.; Liu, Y.-X.; Song, H.-J.; Wang, Q.-M. *Adv. Synth. Catal.* **2020**, *362*, 3110–3115; (e) Tokushige, K.; Kobori, Y.; Asai, S.; Abe, T. *Org. Biomol. Chem.* **2024**, *22*, 7343–7348; (f) Laha, J. K.; Bhimpuria, R. A.; Prajapati, D. V.; Dayal, N.; Sharma, S. *Chem. Commun.* **2016**, *52*, 4329–4332.
- 2) Yamashiro, T.; Abe, T. *Chem. Commun.* **2024**, *60*, 6615–6618.



```

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

```



```

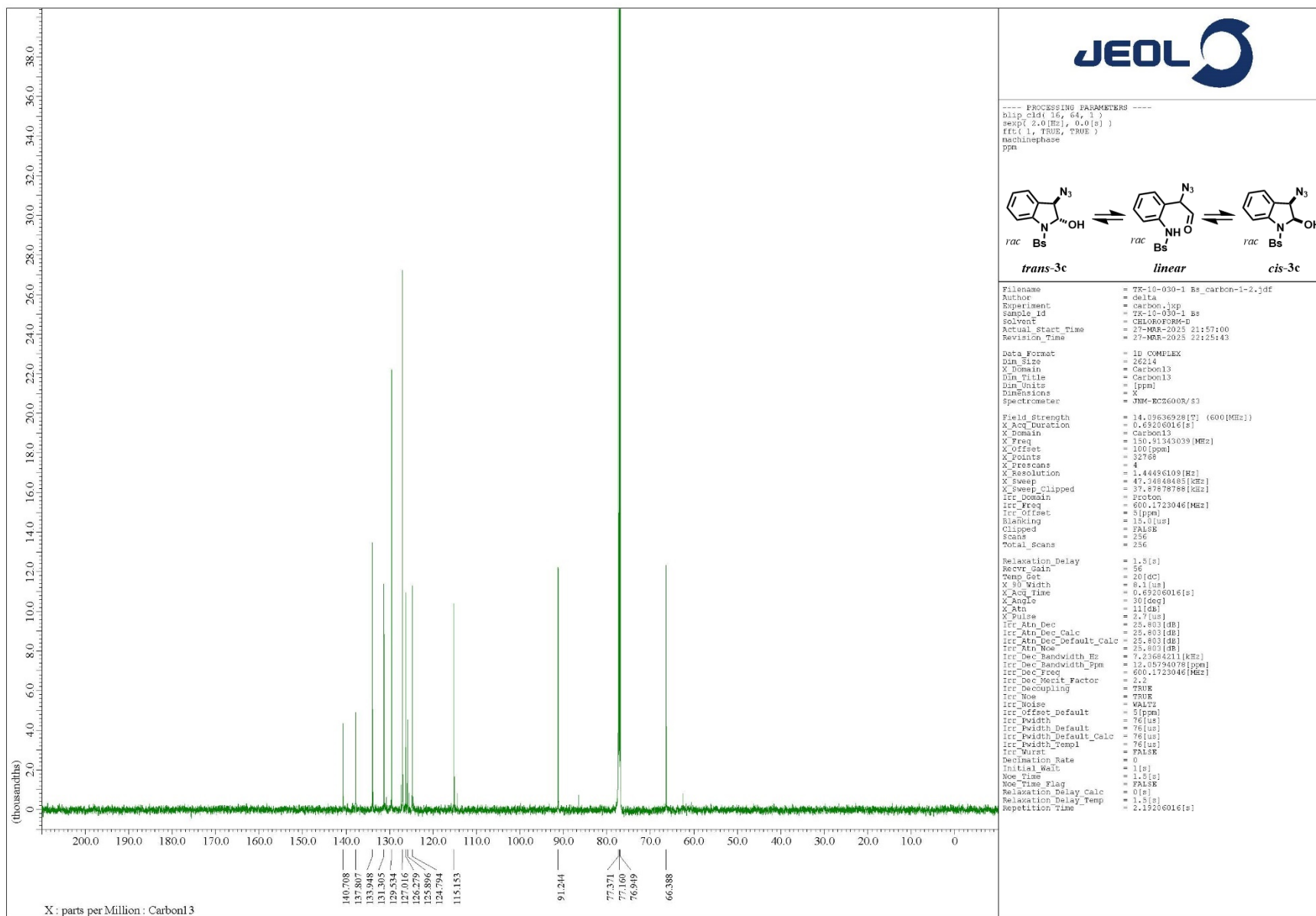
Filename      = TK-10-020-1_Bs_proton-1-3.jdf
Author       = delta
Experiment   = proton_1xp
Sample_Id    = TK-10-020-1_Bs
Solvent      = CHLOROFORM-D
Actual_Start_Time = 27-MAR-2025 21:54:47
Revision_Time   = 27-MAR-2025 22:03:44

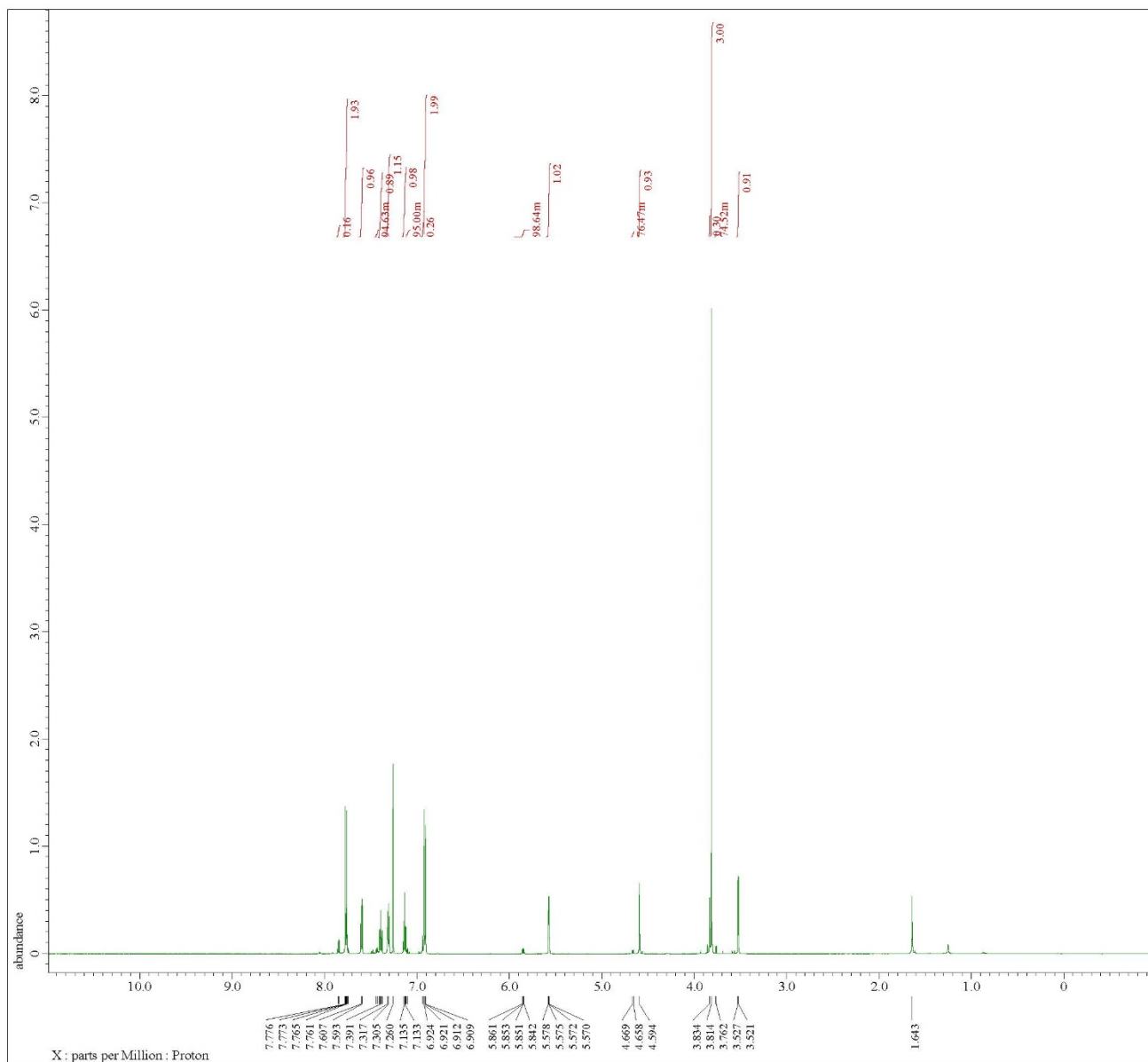
Data_Format   = 1D COMPLEX
Data_Size     = 26214
X_Domain      = Proton
Data_Title    = Proton
Data_Units    = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ600R/S3

Field_Strength = 14.09636328[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain       = Proton
X_Freq         = 600.1723046[MHz]
X_Offset       = 5[ppm]
X_Points       = 32788
X_Prescans     = 1
X_Resolution   = 0.45849727[Hz]
X_Sweep        = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
F1_Freq        = 600.1723046[MHz]
F1_Offset      = 5[ppm]
F1_Domain      = Proton
F1_Freq        = 600.1723046[MHz]
F1_Offset      = 5[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_Scans    = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 46
Temp_Set         = 20[degC]
X_90_Width       = 10.5[us]
X_Acq_Time       = 2.18103808[s]
X_Angle          = 45[deg]
X_Attn           = 8.1[dB]
X_Pulse          = 6.25[us]
F1_Mode          = CFF
F1_Mode         = CFF
Dante_Loop       = ON
Dante_Preset     = FALSE
Decimation_Rate  = 0
Initial_Wait     = 1[s]
Phase            = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time      = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time  = 4.18103808[s]

```

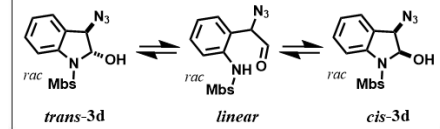




```

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

```



```

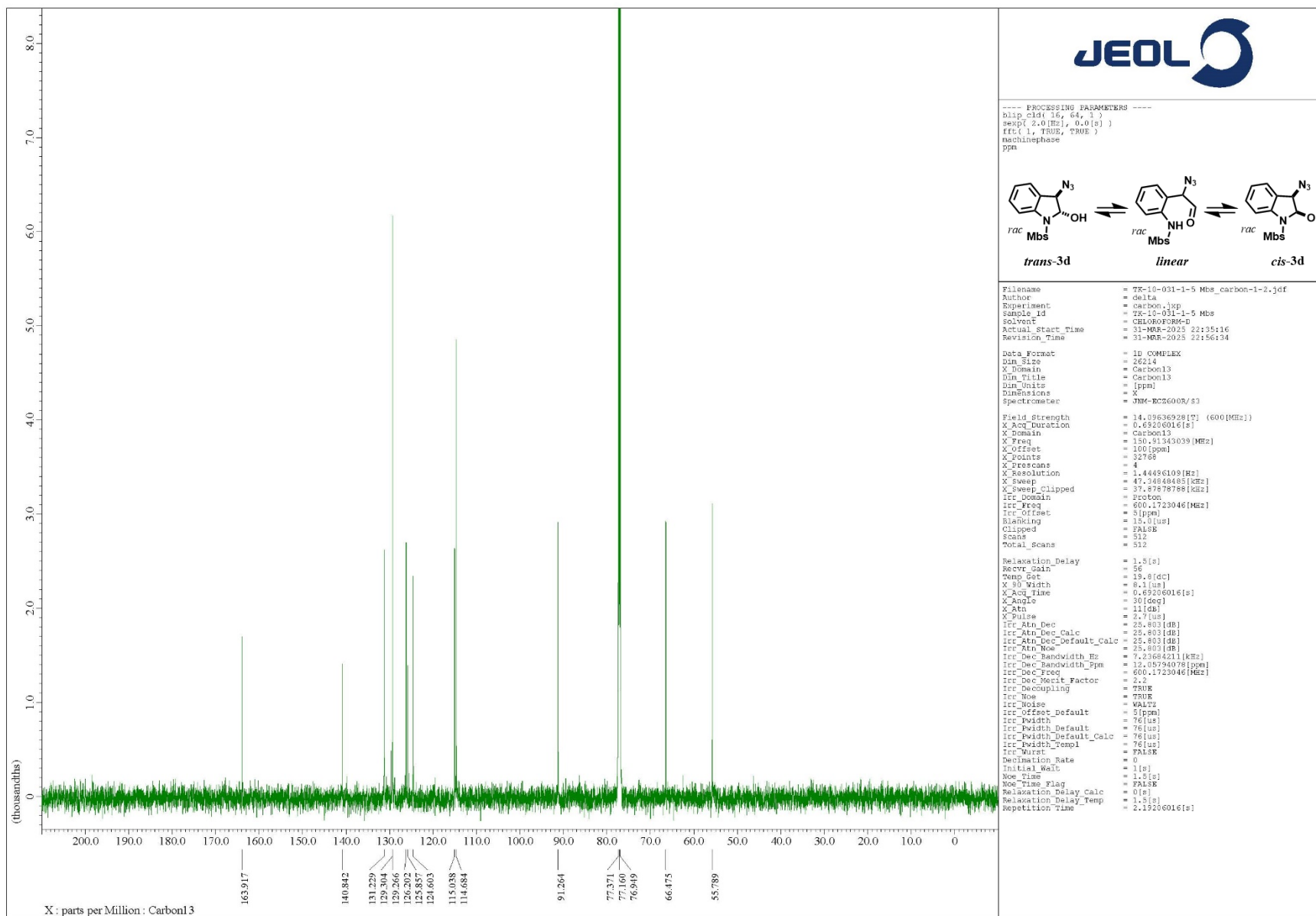
Filename      = TK-10-031-1-5 Mbs_proton-1-3.jdf
Author        = Delta
Experiment    = proton_3xp
Sample_id     = TK-10-031-1-5 Mbs
Solvent       = CHLOROFORM-D
Actual_Start_Time = 31-MAR-2025 22:34:21
Revision_Time = 1-APR-2025 09:00:06

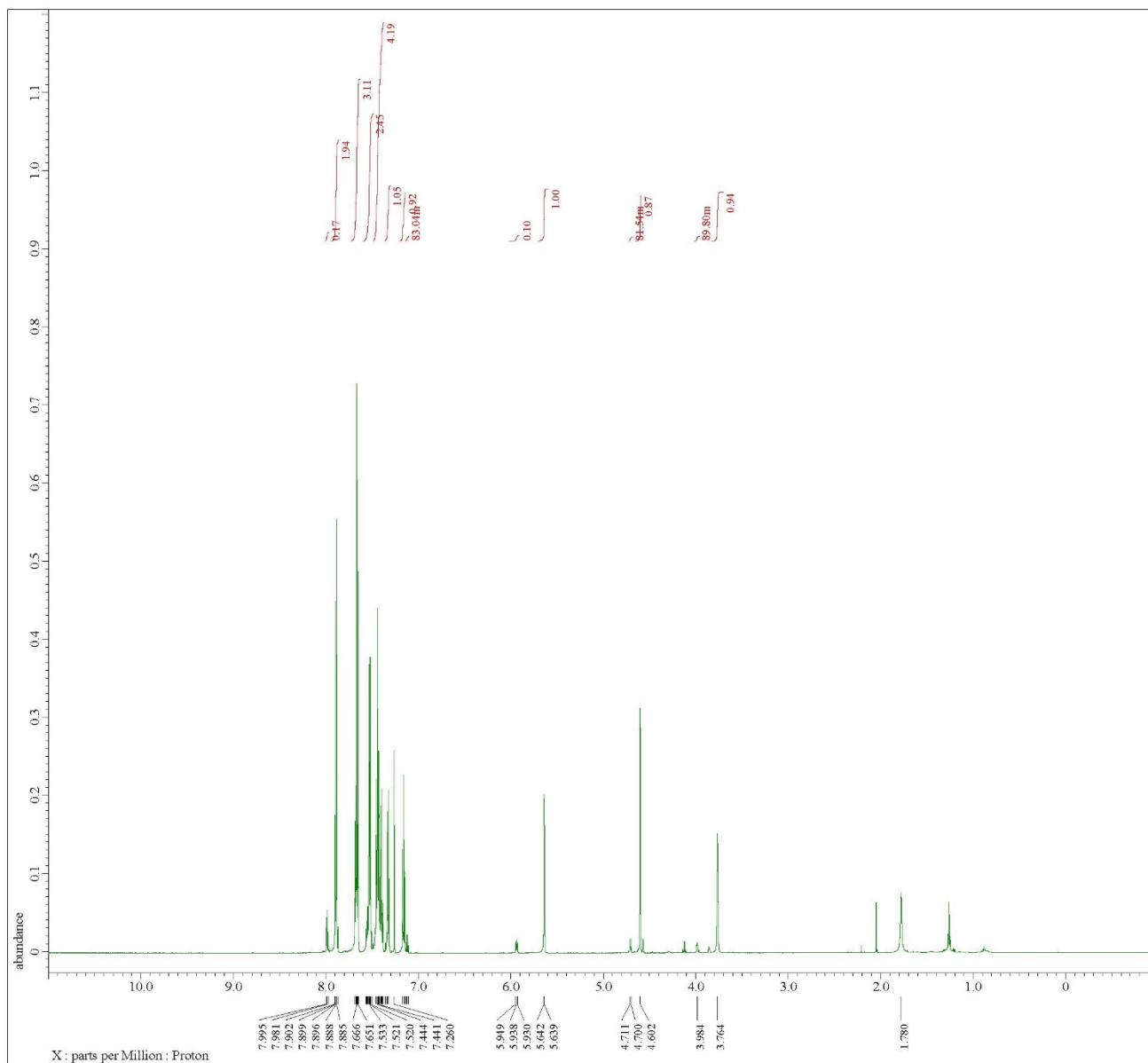
Data_Format   = 1D COMPLEX
Din_Size      = 26214
X_Domain      = Proton
Din_Title     = Proton
Din_Units     = [ppm]
Dimensions    = 2
Spectrometer  = JNM-ECZ600R/S3

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain       = Proton
X_Freq         = 600.1723046[MHz]
X_Offset       = 8[ppm]
X_Points       = 32768
X_Prescans     = 1
X_Resolution   = 0.45849727[Hz]
X_Sweep        = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
F1_Domain      = Proton
F1_Freq        = 600.1723046[MHz]
F1_Offset      = 8[ppm]
Tc1_Domain     = Proton
Tc1_Freq       = 600.1723046[MHz]
Tc1_Offset     = 8[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_Scans    = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 56
Temp_Set        = 19.7[degC]
X_90_Width      = 10.5[us]
X_Acq_Time      = 2.18103808[s]
X_Angle         = 45[deg]
X_Atn           = 8.1[ds]
X_Pulse         = 8.25[us]
F1_Mode         = off
Tc1_Mode        = off
Dante_Loop      = 200
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Walt    = 1[s]
Phase           = {0, 90, 270, 180, 180, 270, 90, 0}
Preset_Time     = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18103808[s]

```

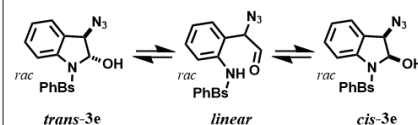




```

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

```



```

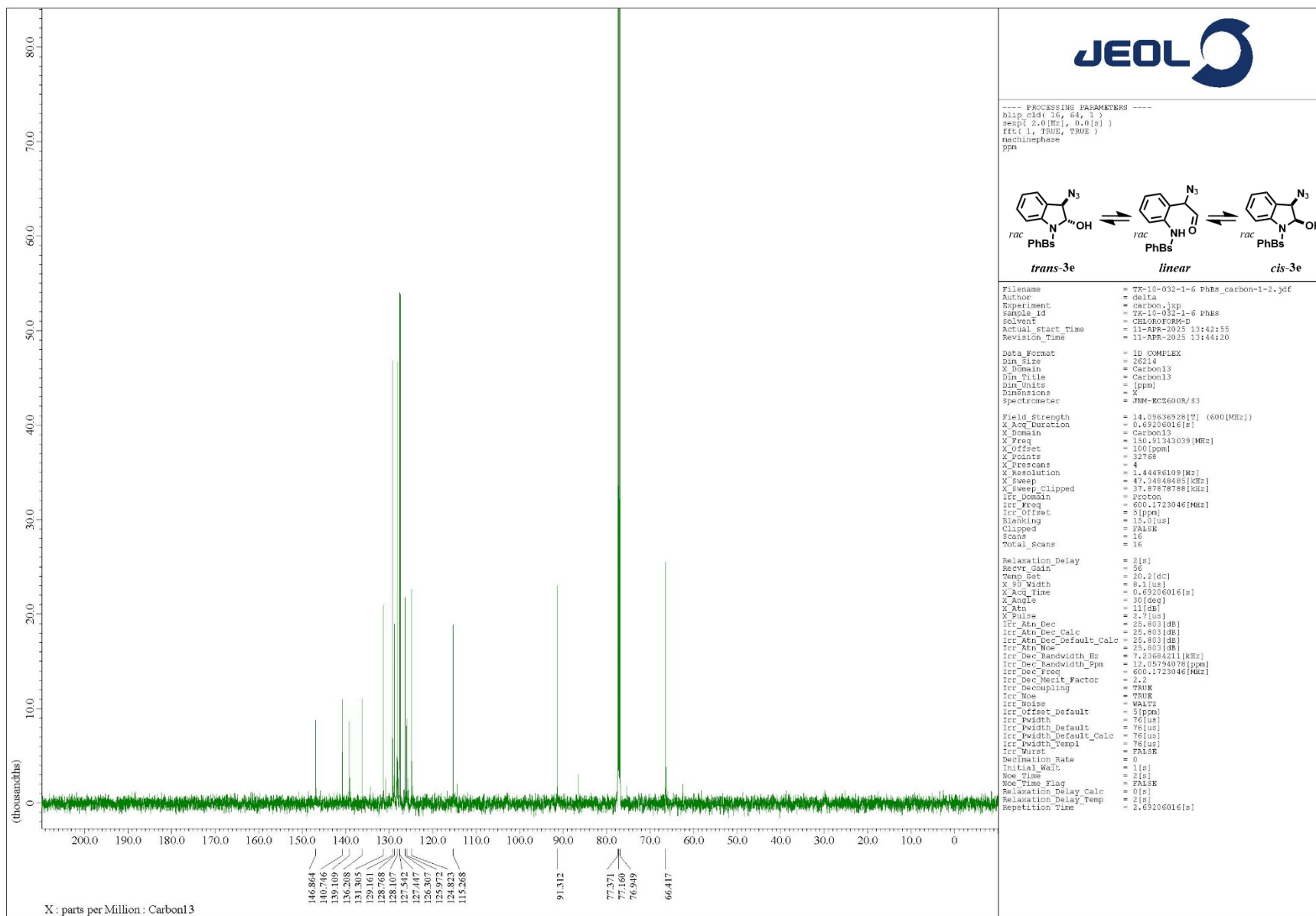
Filename      = TK-10-032-1-6 PhBs_proton-1-3.jdf
Author        = delta
Experiment    = proton_3xp
Sample_id     = TK-10-032-1-6 PhBs
Solvent       = CHLOROFORM-D
Actual_Start_Time = 11-APR-2025 13:44:22
Revision_Time = 11-APR-2025 14:35:07

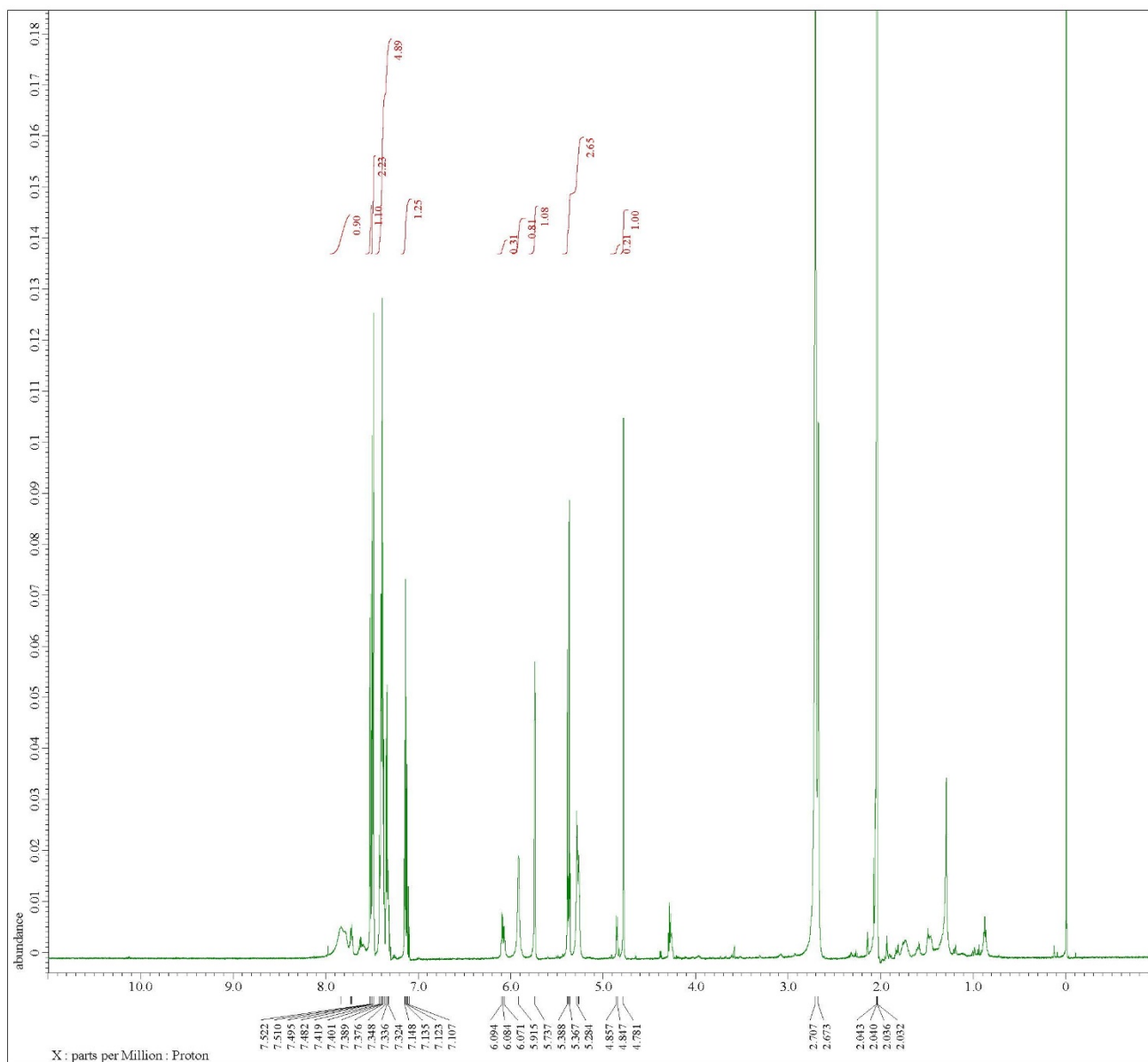
Data Format    = 1D COMPLEX
Dim Size      = 32768
X_Domain      = Proton
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ600R/S3

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]
F1_Domain      = Proton
F1_Freq        = 600.1723046[MHz]
F1_Offset      = 5[ppm]
T1_Domain      = Proton
T1_Freq        = 600.1723046[MHz]
T1_Offset      = 5[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_Scans    = 4

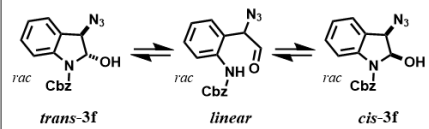
Relaxation_Delay = 2[s]
Recvr_Gain       = 36
Temp_Set         = 20.2[degC]
X_90_Width       = 10.5[us]
X_Acq_Time       = 2.90455552[s]
X_Angle          = 45[deg]
X_Atn            = 8.1[db]
X_Pulse          = 8.25[us]
T1F_Mode         = Off
T1F_Mode         = Off
Dante_Loop       = 200
Dante_Preset     = FALSE
Decimation_Rate  = 0
Initial_Walt     = 1[s]
Phase            = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time      = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time  = 4.90455552[s]

```

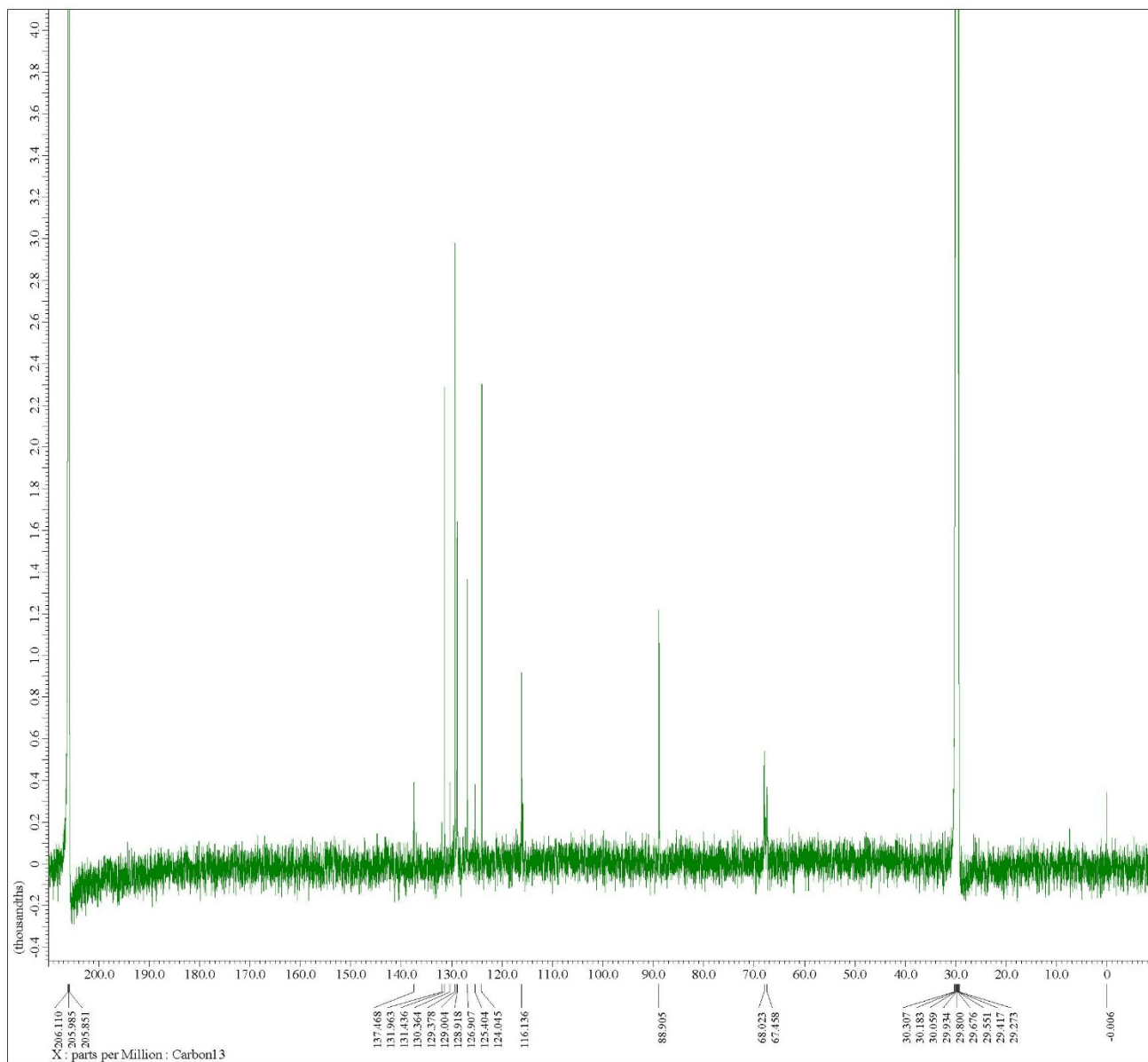




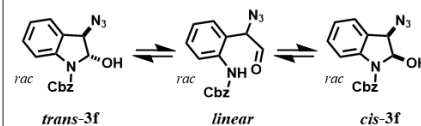
----- PROCESSING PARAMETERS -----
sexpr(0.2[Hz], 0.01[Hz])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm



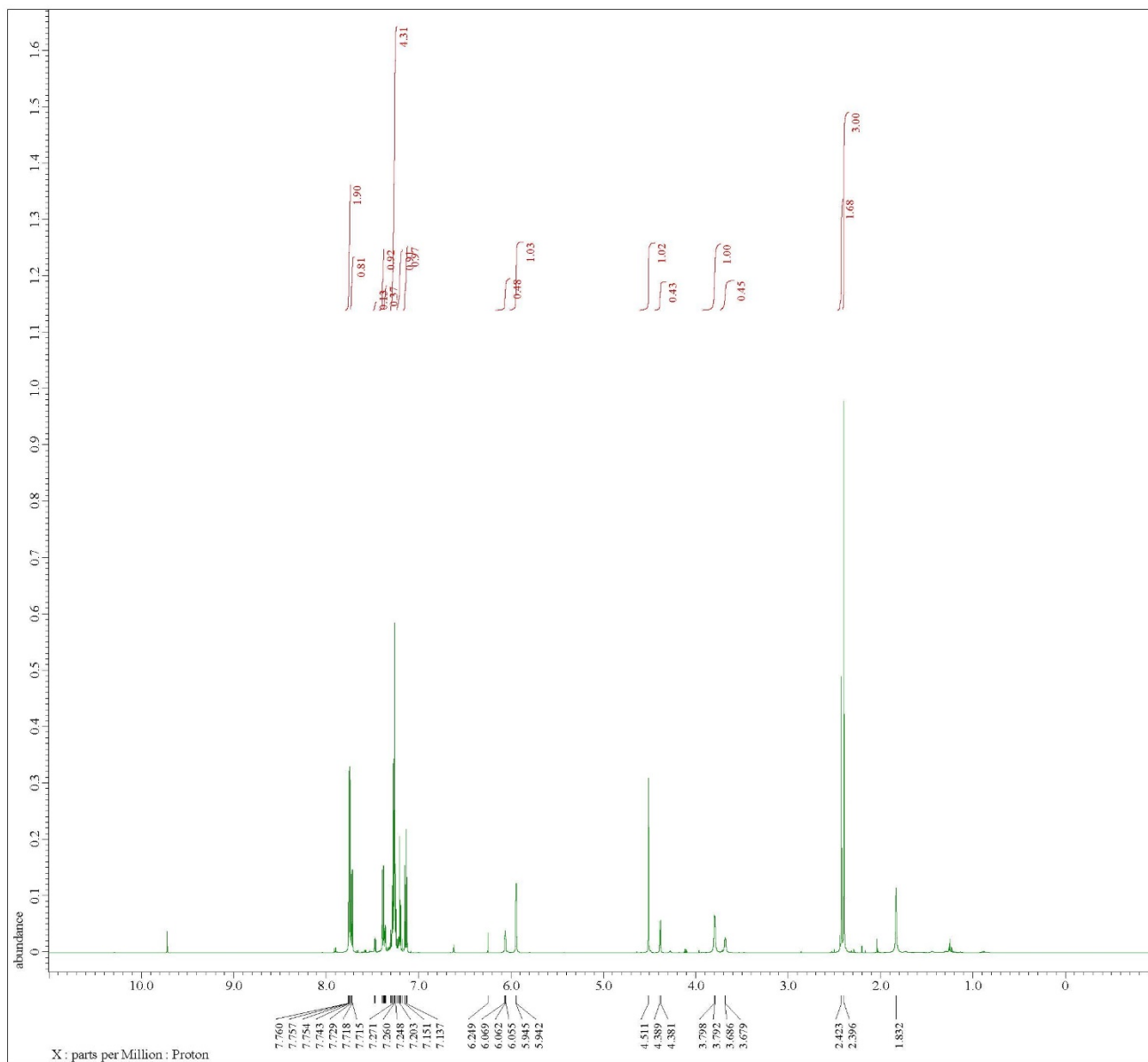
Filename = TK-10-033-PTLC_proton-1-3.jdf
Author = Delta
Experiment = proton.jpg
Sample_id = TK-10-033-PTLC
Solvent = ACETONE-d6
Actual_Start_Time = 30-MAY-2025 11:06:27
Revision_Time = 30-MAY-2025 12:13:20
Data_Format = 1D COMPLEX
Dm_Size = 26214
X_Domain = Proton
Dm_Title = Proton
Dm_Units = [ppm]
Dimensions = 2
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 = 15.02402946[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tcl_Domain = Proton
Tcl_Freq = 600.1723046[MHz]
Tcl_Offset = 5[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 2[s]
Recvr_Gain = 46
Temp_Set = 40[degC]
X_90_Width = 10.5[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 8.1[deg]
X_Pulse = 5.25[us]
Irr_Mode = off
Tcl_Mode = off
Dante_Loop = 200
Dante_Preset = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18103808[s]



----- PROCESSING PARAMETERS -----
 blp.cld(16, 64, 1)
 sepf(2.0[Hz], 0.0[s])
 fft(1, TRUE, TRUE)
 nucleus=c
 ppn



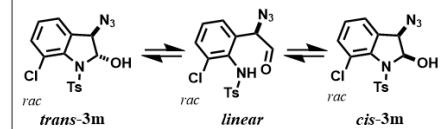
Filename = TK-10-033-PTLC_carbon-1-3.jdf
 Author = delta
 Experiment = carbon-13p
 Sample_id = TK-10-033-PTLC
 Solvent = ACETONE-d6
 Actual_Start_Time = 30-MAY-2025 11:09:02
 Revision_Time = 30-MAY-2025 12:20:16
 Data_Format = 1D REAL
 Dm_Size = 26214
 X_Domain = Carbon13
 Dm_Title = Carbon13
 Dm_Units = [ppm]
 Dimensions = 1
 Spectrometer = JNM-ECP600R/53
 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]
 Y_Sweep = 47.34848485[kHz]
 X_Sweep_Clippped = 37.87878788[kHz]
 Irc_Domain = Proton
 Irc_Freq = 600.1723046[MHz]
 Irc_Offset = 5[ppm]
 Blanking = 15.0[us]
 Clipped = FALSE
 Scans = 1024
 Total_Scans = 1024
 Relaxation_Delay = 1.5[s]
 Recvr_Gain = 56
 Temp_Gst = 40[deg]
 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]
 Irc_Atn_Dec = 25.803[db]
 Irc_Atn_Dec_Calc = 25.803[db]
 Irc_Atn_Dec_Default_Calc = 25.803[db]
 Irc_Atn_Noise = 25.803[db]
 Irc_Dec_Bandwidth_Hz = 7.23664211[kHz]
 Irc_Dec_Bandwidth_Fpm = 12.05794078[ppm]
 Irc_Dec_Freq = 600.1723046[MHz]
 Irc_Dec_Merit_Factor = 2.2
 Irc_Decoupling = TRUE
 Irc_Noise = TRUE
 Irc_Noise = WALTZ
 Irc_Offset_Default = 5[ppm]
 Irc_Pwidth = 76[us]
 Irc_Pwidth_Default = 76[us]
 Irc_Pwidth_Default_Calc = 76[us]
 Irc_Pwidth_Templ = 76[us]
 Irc_Wurst = FALSE
 Decoupling_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 = 2.37206016[s]



```

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

```



```

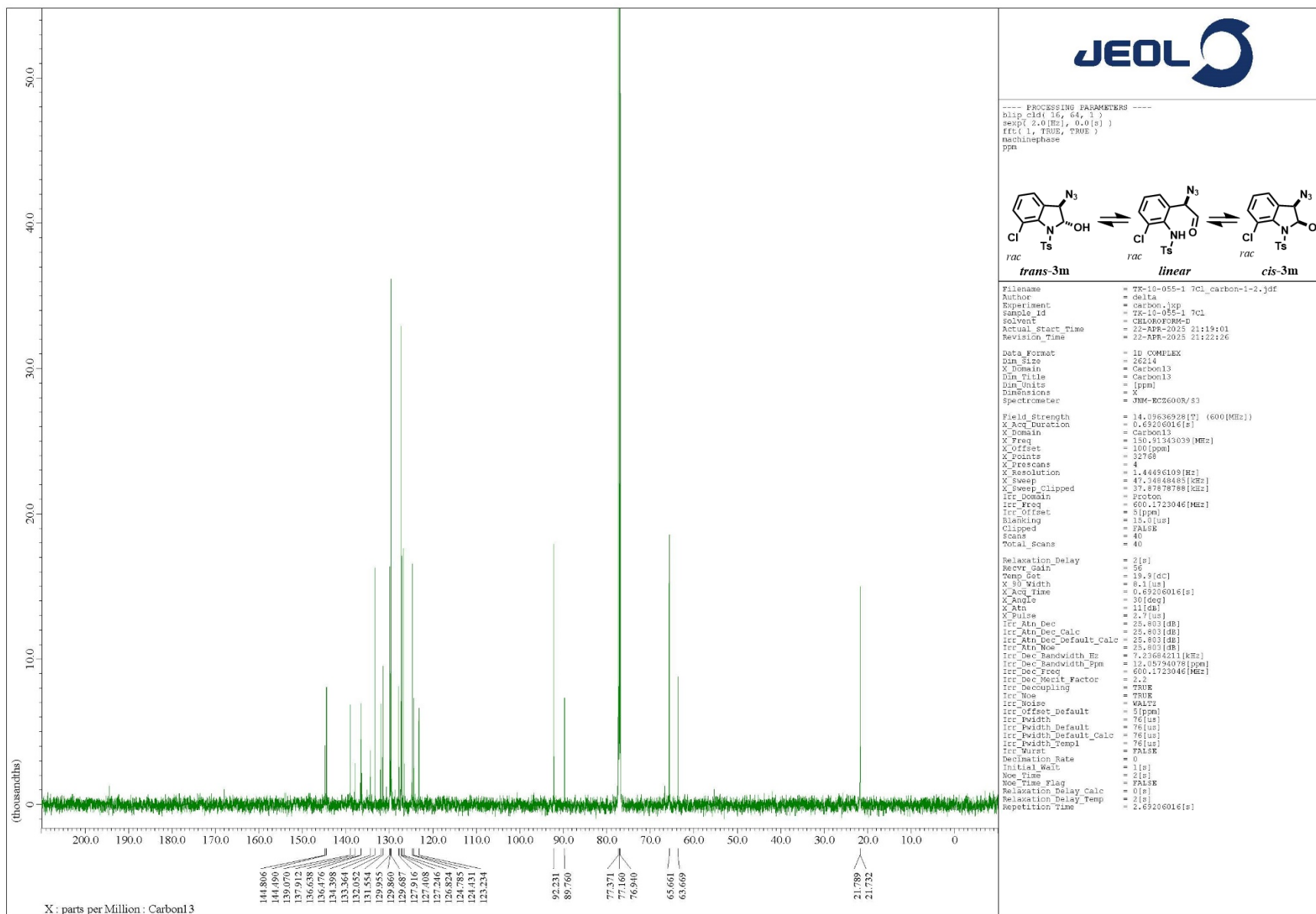
Filename      = TK-10-055-1 7c1_proton-1-3.jdf
Author        = delta
Experiment    = proton_1xp
Sample_id     = TK-10-055-1 7c1
Solvent       = CHLOROFORM-D
Actual_Start_Time = 22-APR-2025 21:16:46
Revision_Time = 27-MAY-2025 12:23:23

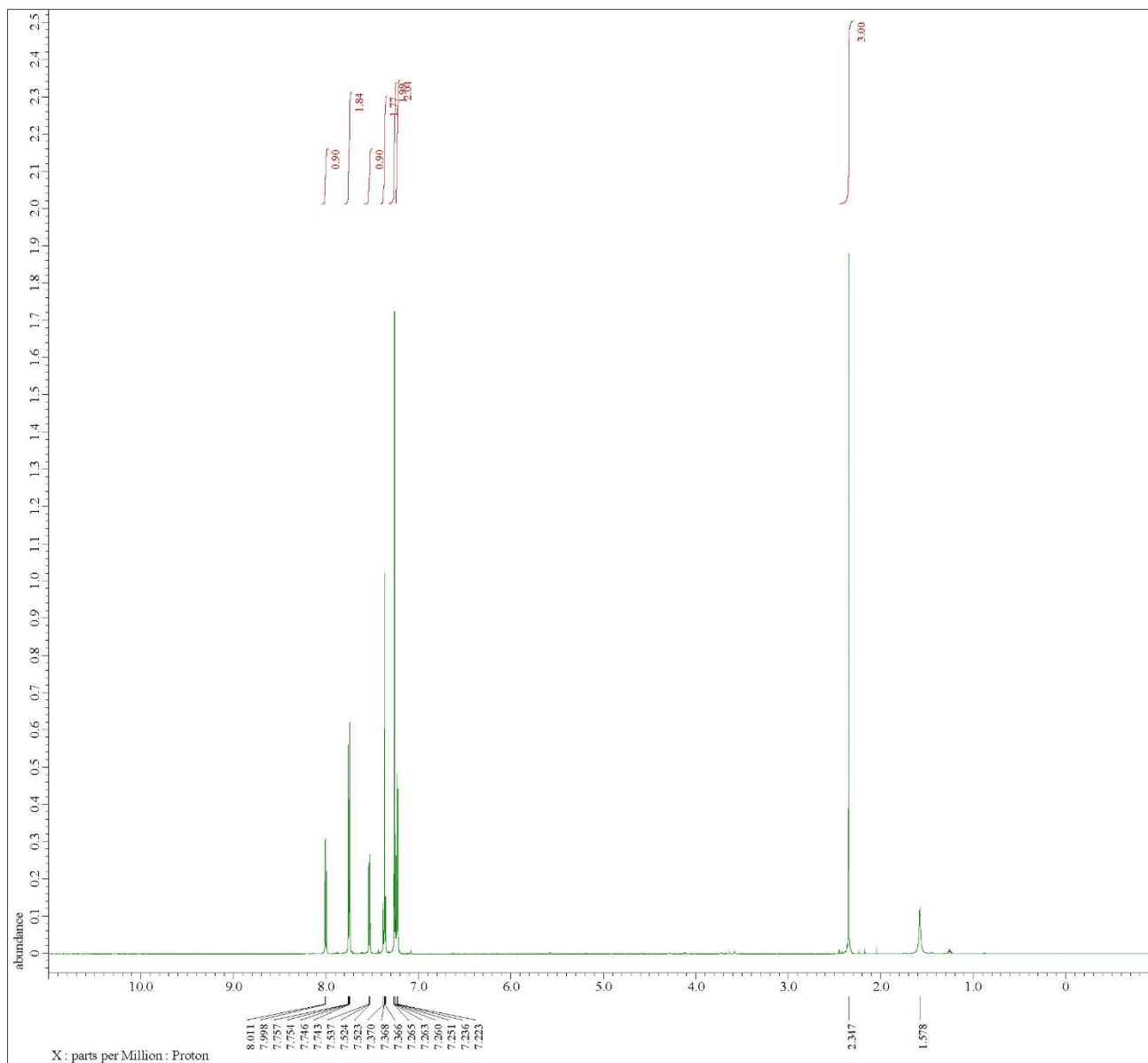
Data Format    = 1D COMPLEX
Dim Size      = 36214
X_Domain      = Proton
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = 1
Spectrometer  = JNM-ECZ600R/S3

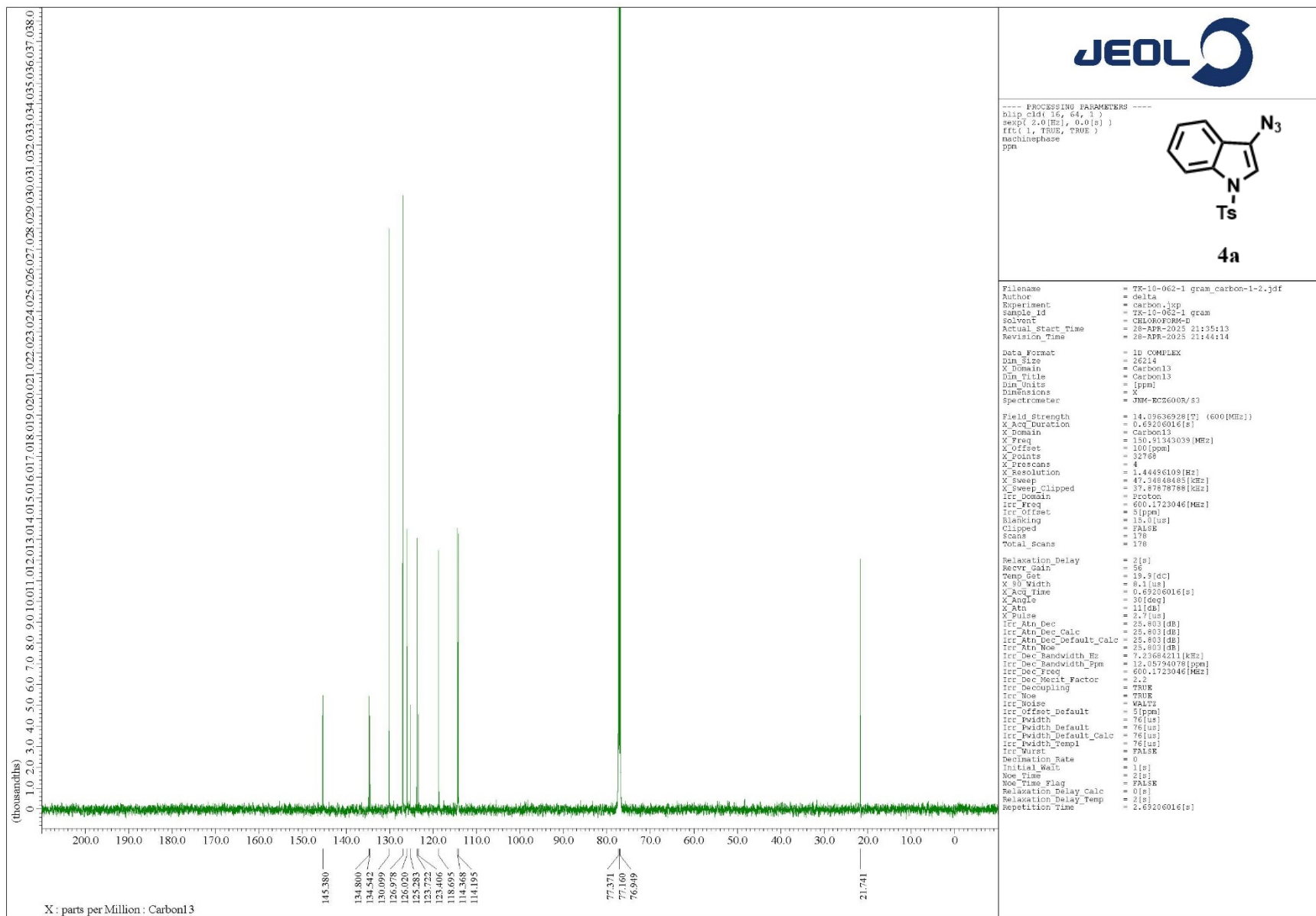
Field Strength = 14.09636928[T] (600[MHz])
X_Acq Duration = 2.18103808[s]
X_Domain      = Proton
X_Freq        = 600.1723046[MHz]
X_Offset      = 8[ppm]
X_Points      = 32768
X_Prescans    = 1
X_Resolution  = 0.43849727[Hz]
X_Sweep       = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
F1 Domain     = Proton
F1 Freq       = 600.1723046[MHz]
F1 Offset     = 8[ppm]
F2 Domain     = Proton
F2 Freq       = 600.1723046[MHz]
F2 Offset     = 5[ppm]
Blanking      = 5.0[us]
Clipped       = FALSE
Scans         = 4
Total_Scans   = 4

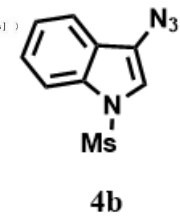
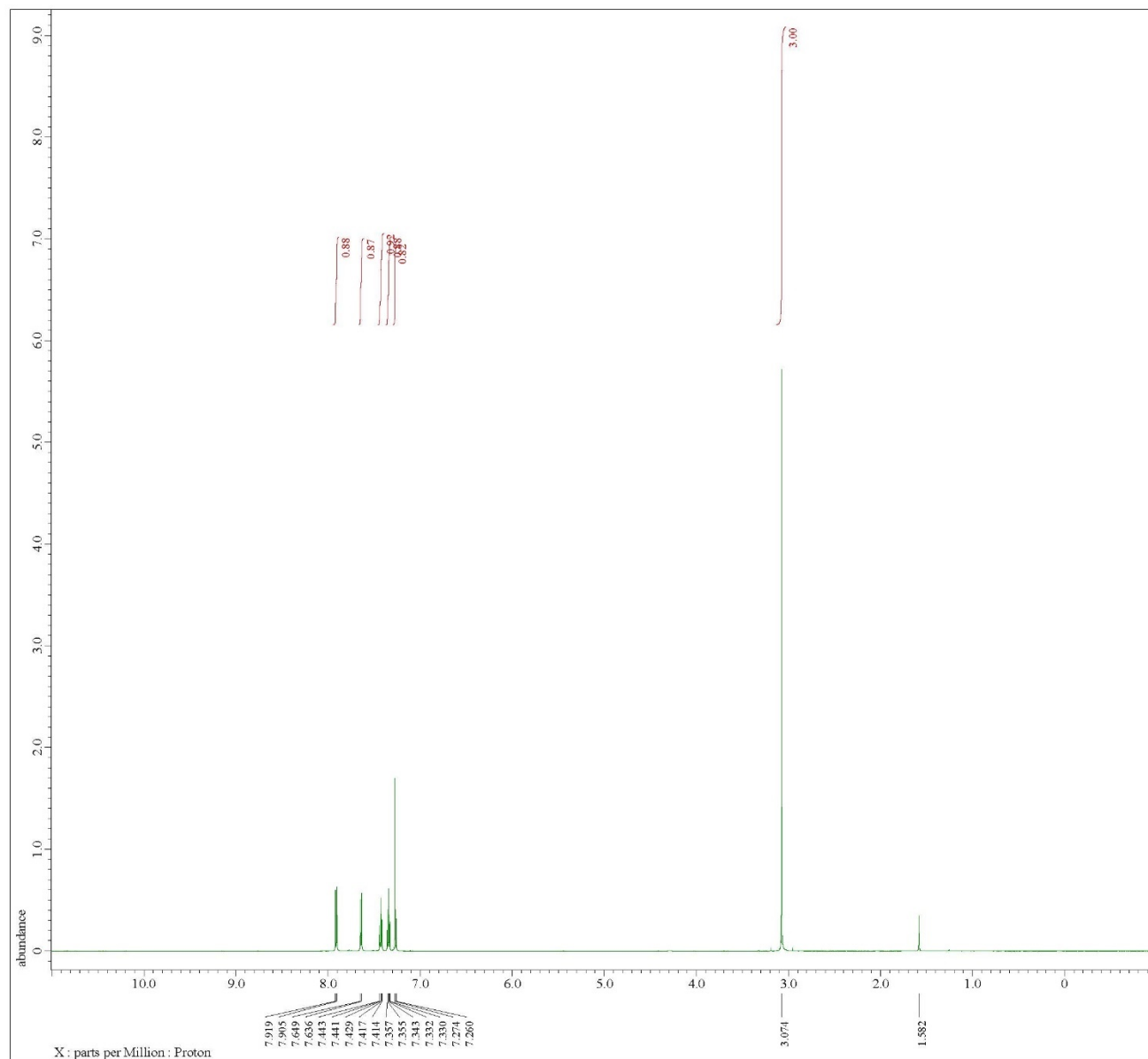
Relaxation_Delay = 2[s]
Recvr Gain      = 36
Temp_Set        = 19.9[degC]
X_90_Width      = 10.5[us]
X_Acq Time      = 2.18103808[s]
X_Angle         = 45[deg]
X_Attn          = 8.1[dB]
X_Pulse         = 6.25[us]
TEC Mode       = Off
TEC Mode       = Off
Dante Loop     = 200
Dante_Preset   = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase          = {0, 90, 270, 180, 180, 270, 90, 0}
Preset_Time     = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18103808[s]

```







```

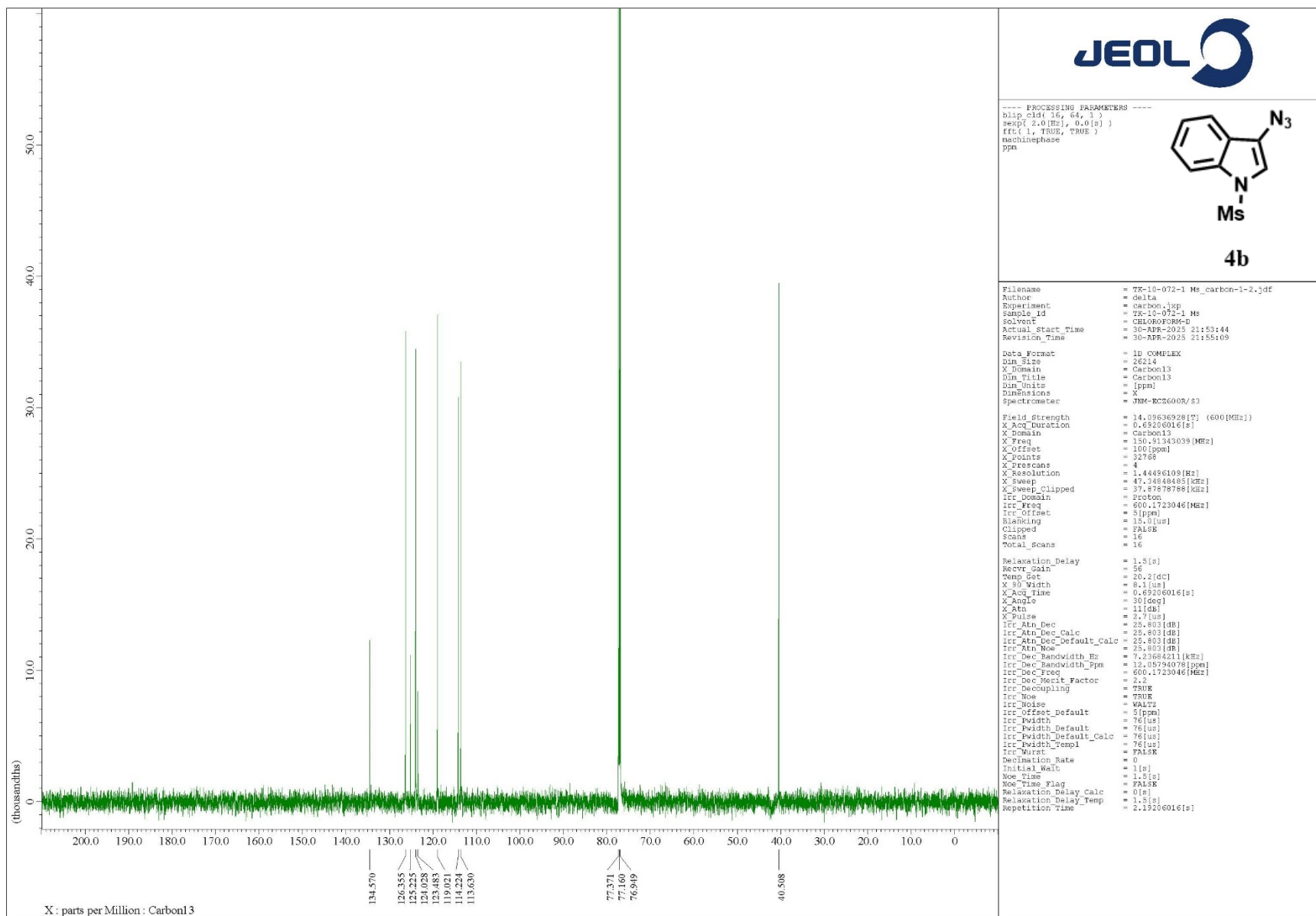
---- PROCESSING PARAMETERS ----
sexpr( 0.2[Hz], 0.01[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

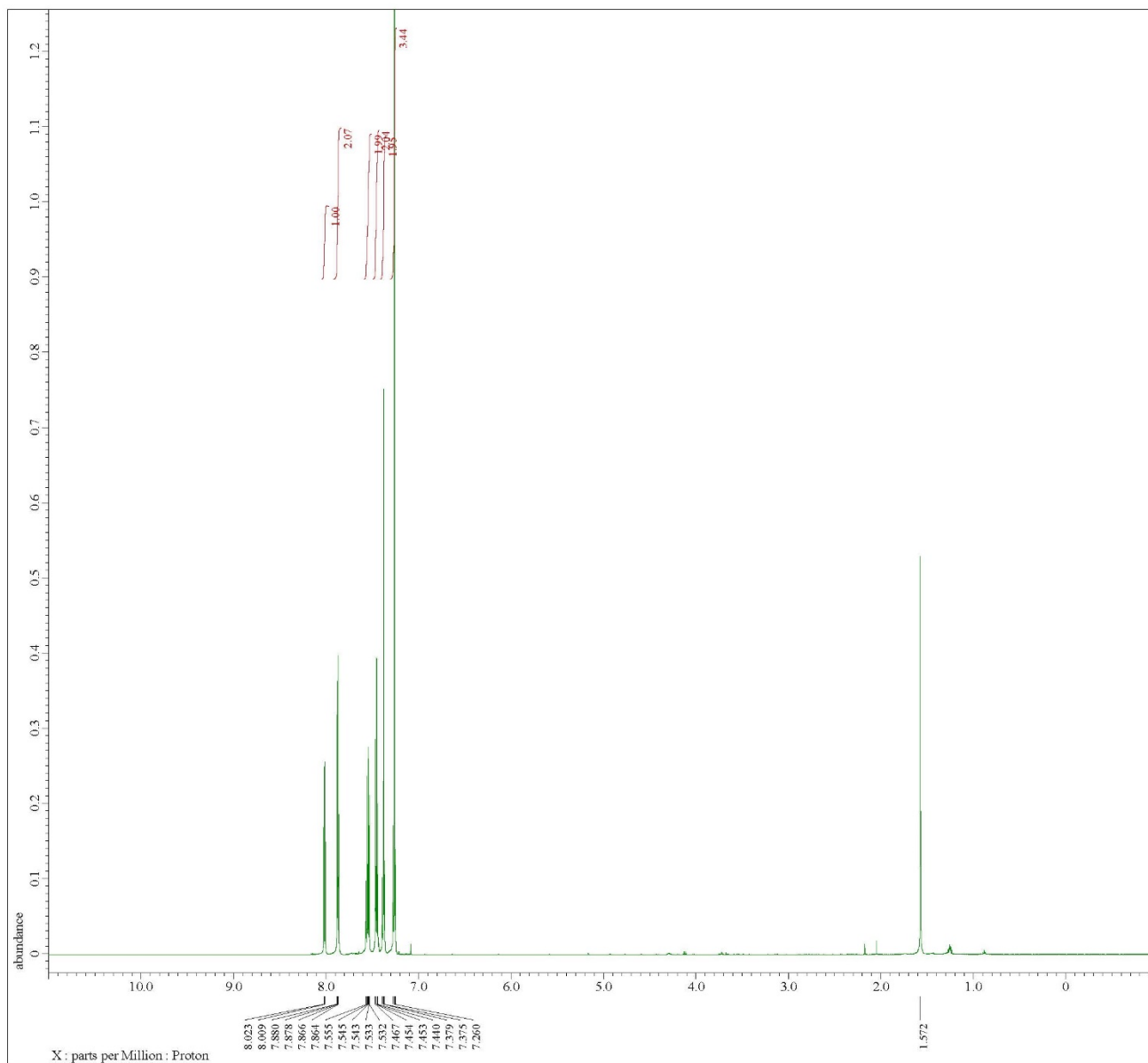
Filename      = TK-10-072-1 Ms_proton-1-3.jdf
Author        = Delta
Experiment    = proton_3xp
Sample_id     = TK-10-072-1 Ms
Solvent       = CHLOROFORM-D
Actual_Start_Time = 30-APR-2025 21:52:46
Revision_Time = 1-MAY-2025 22:30:22

Data_Format   = 1D COMPLEX
Din_Size      = 26214
X_Domain      = Proton
Din_Title     = Proton
Din_Units     = [ppm]
Dimensions    = 2
Spectrometer  = JNM-ECZ600R/S3

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain       = Proton
X_Freq         = 600.1723046[MHz]
X_Offset       = 8[ppm]
X_Points       = 32768
X_Prescans     = 1
X_Resolution   = 0.45849727[Hz]
X_Sweep        = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
Ict_Domain     = Proton
Ict_Freq       = 600.1723046[MHz]
Ict_Offset     = 8[ppm]
Tcl_Domain     = Proton
Tcl_Freq       = 600.1723046[MHz]
Tcl_Offset     = 8[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_scans    = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 46
Temp_Set         = 20.4[degC]
X_90_Width       = 10.3[us]
X_Acq_Time       = 2.18103808[s]
X_Angle          = 45[deg]
X_Atn            = 8.1[ds]
X_Pulse          = 8.25[us]
Prg_Mode         = off
Tcl_Mode         = off
Dante_Loop       = 200
Dante_Preset     = FALSE
Decimation_Rate  = 0
Initial_Walt     = 1[s]
Phase            = {0, 90, 270, 180, 180, 270, 90, 0}
Preset_Time      = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time  = 4.18103808[s]
  
```

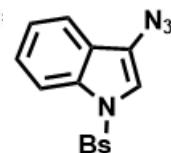




```

---- PROCESSING PARAMETERS ----
sext( 0.2[Hz], 0.0[F] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinphase
ppm

```



4c

```

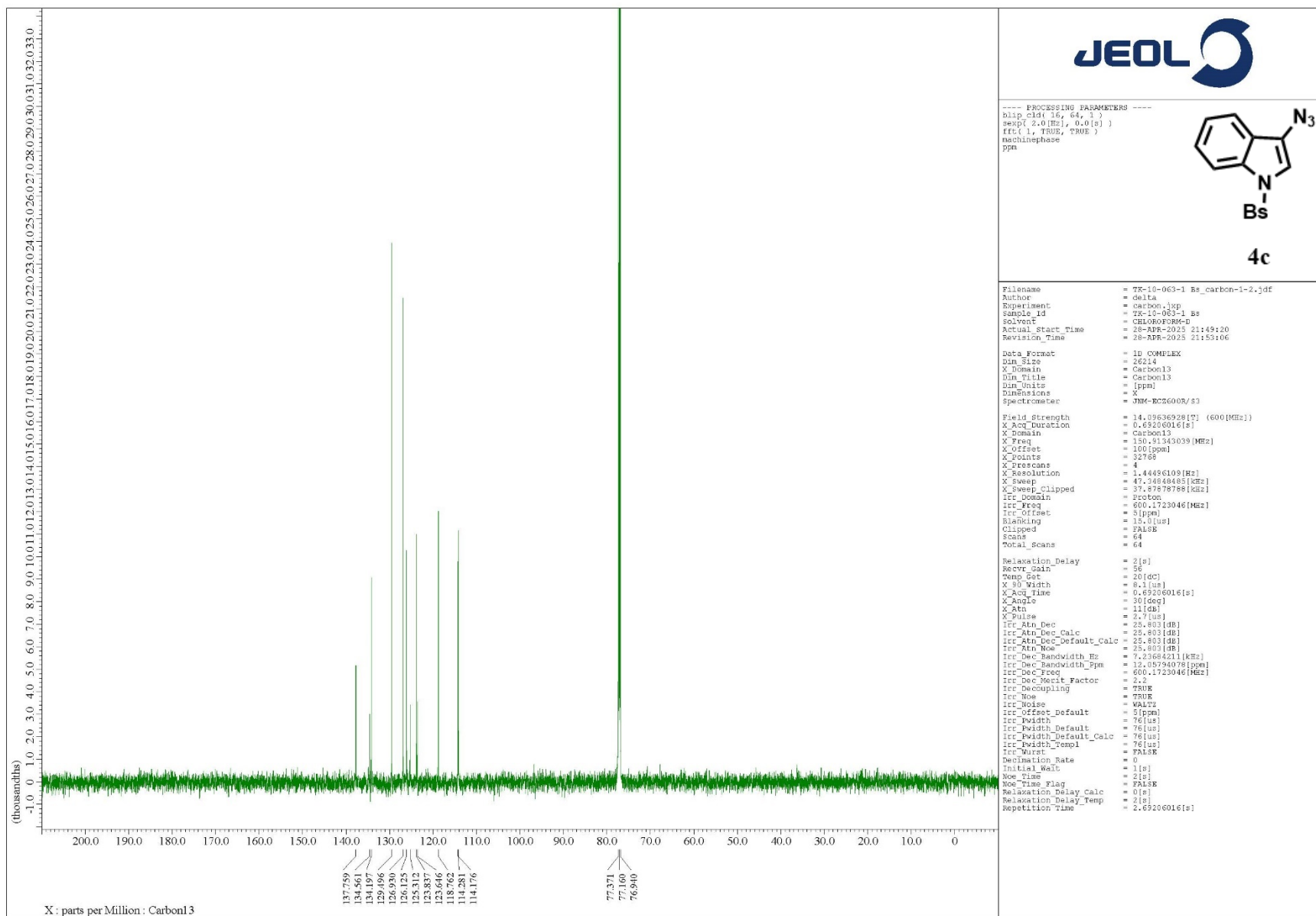
Filename      = TK-10-063-1 Bs_proton-1-5.jdf
Author        = delta
Experiment    = proton_3xp
Sample_id     = TK-10-063-1 Bs
Solvent       = CHLOROFORM-D
Actual_Start_Time = 28-APR-2025 21:48:16
Revision_Time = 28-APR-2025 22:58:52

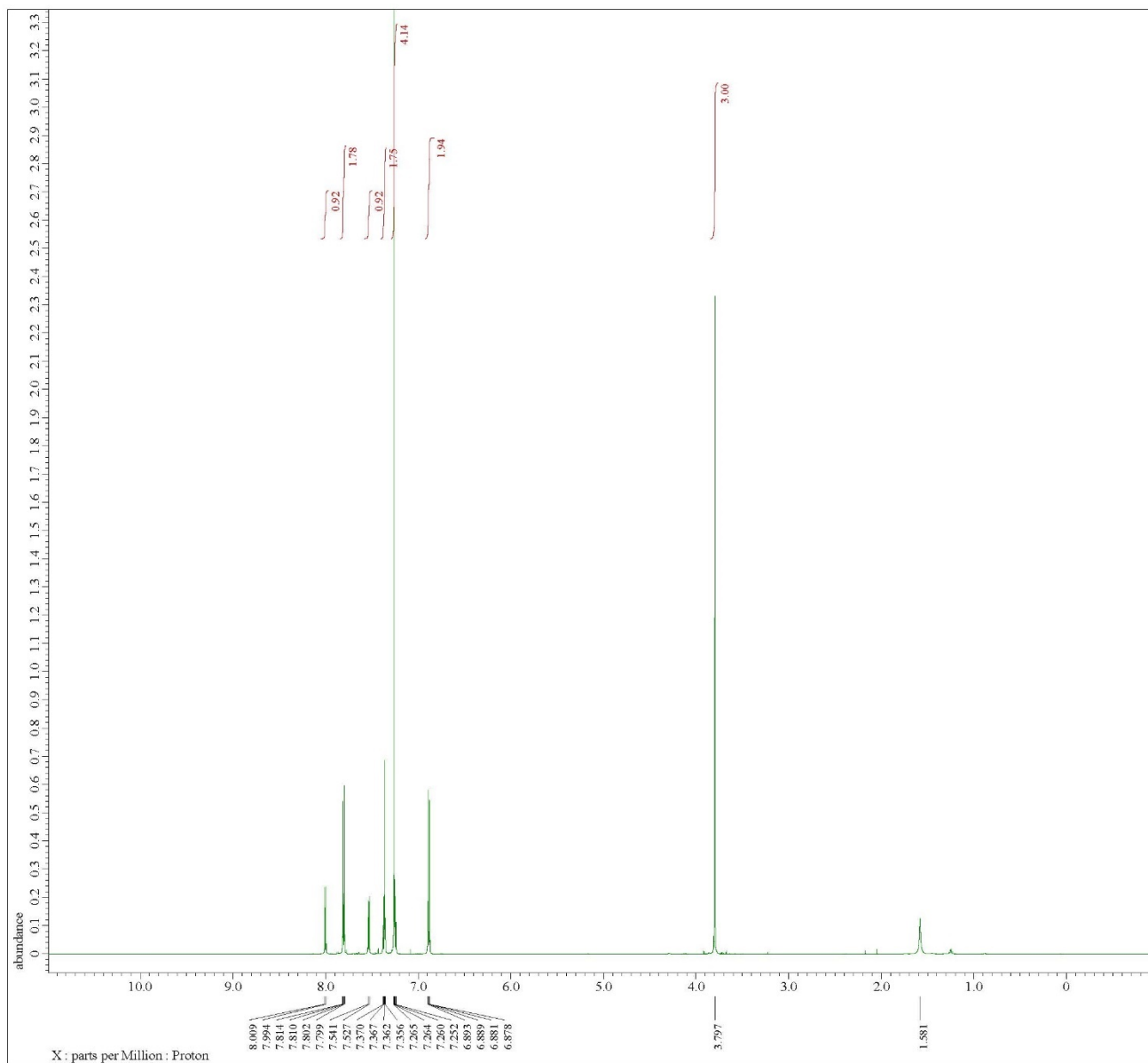
Data Format    = 1D COMPLEX
Dim Size      = 32768
X_Domain      = Proton
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = 1
Spectrometer  = JNM-ECZ600R/S3

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]
Y_Sweep       = 11.28158845[kHz]
X_Sweep_Clip  = 0.02527076[kHz]
F1_Domain     = Proton
F1_Freq       = 600.1723046[MHz]
F1_Offset     = 5[ppm]
T1_Domain     = Proton
T1_Freq       = 600.1723046[MHz]
T1_Offset     = 5[ppm]
Blanking      = 5.0[us]
Clipped       = FALSE
Scans         = 4
Total_Scans   = 4

Relaxation_Delay = 2[s]
Recvr Gain      = 46
Temp_Set        = 19.9[degC]
X_90_Width      = 10.5[us]
X_Acq Time      = 2.90455552[s]
X_Angle         = 45[deg]
X_Atn           = 8.1[db]
X_Pulse         = 8.25[us]
T1c Mode        = Off
T1c Loop        = Off
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Waltz   = 1[s]
Phase           = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time     = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition Time = 4.90455552[s]

```

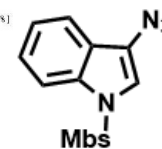




```

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

```



4d

```

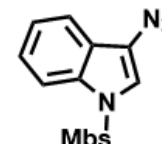
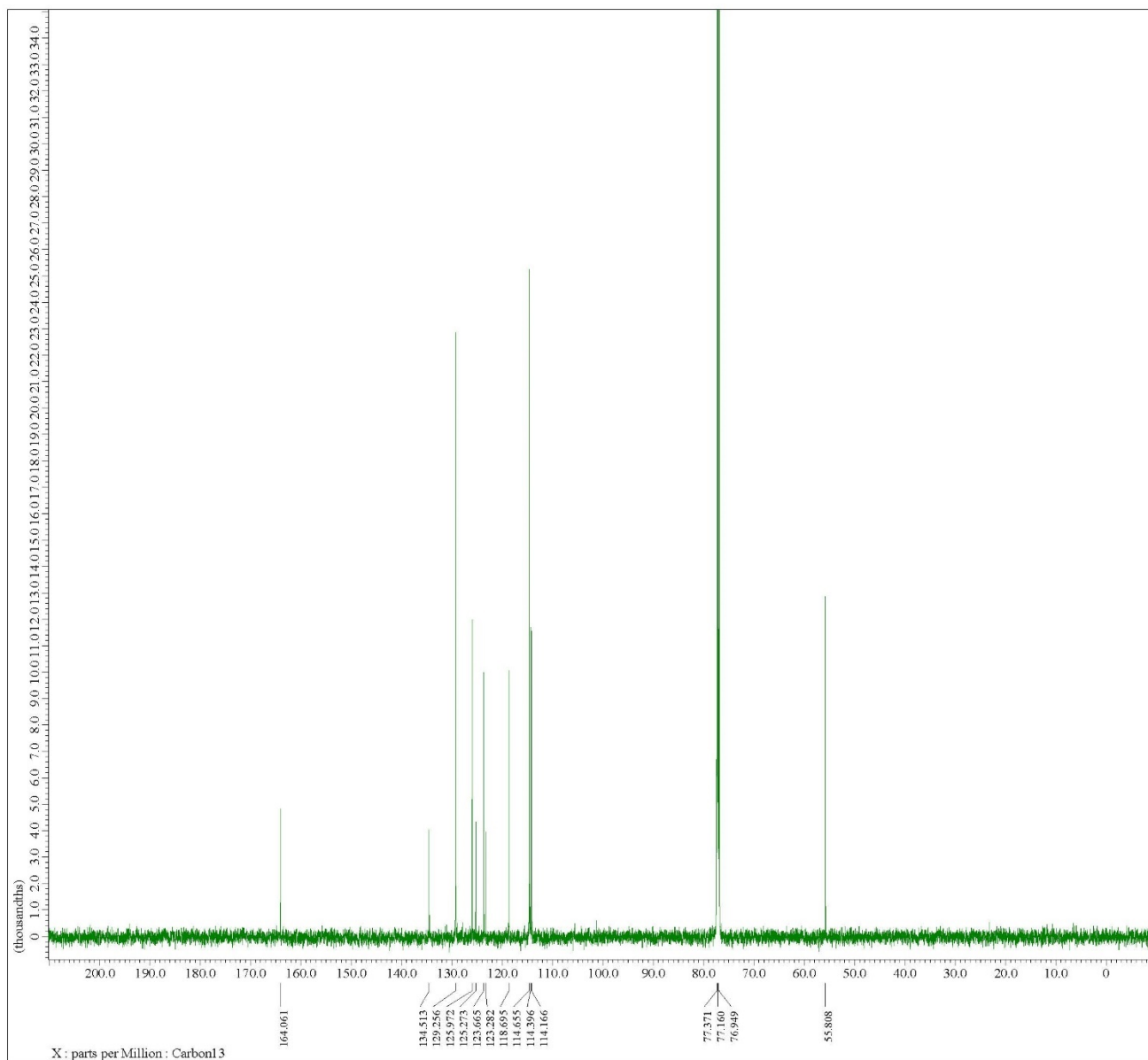
Filename      = TK-10-064-1 Mbs_proton-1-3.jdf
Author        = delta
Experiment    = proton_3xp
Sample_id     = TK-10-064-1 Mbs
Solvent       = CHLOROFORM-D
Actual_Start_Time = 28-APR-2025 21:58:09
Revision_Time = 28-APR-2025 23:02:09

Data_Format   = 1D COMPLEX
Data_Size     = 26214
X_Domain      = Proton
Data_Title    = Proton
Data_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]
Y_Domain       = Proton
Y_Freq         = 600.1723046[MHz]
Y_Offset       = 5[ppm]
Y1_Domain      = Proton
Y1_Freq        = 600.1723046[MHz]
Y1_Offset      = 5[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_Scans    = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 46
Temp_Set         = 19.5[degC]
X_90_Width       = 10.5[us]
X_Acq_Time       = 2.90455552[s]
X_Angle          = 45[deg]
X_Atn            = 8.1[db]
X_Pulse          = 8.25[us]
TFR_Mode        = Off
TFR1_Mode        = Off
Dante_Loop       = 200
Dante_Preset     = FALSE
Decimation_Rate  = 0
Initial_Walt     = 1[s]
Phase            = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time      = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time  = 4.90455552[s]

```



4d

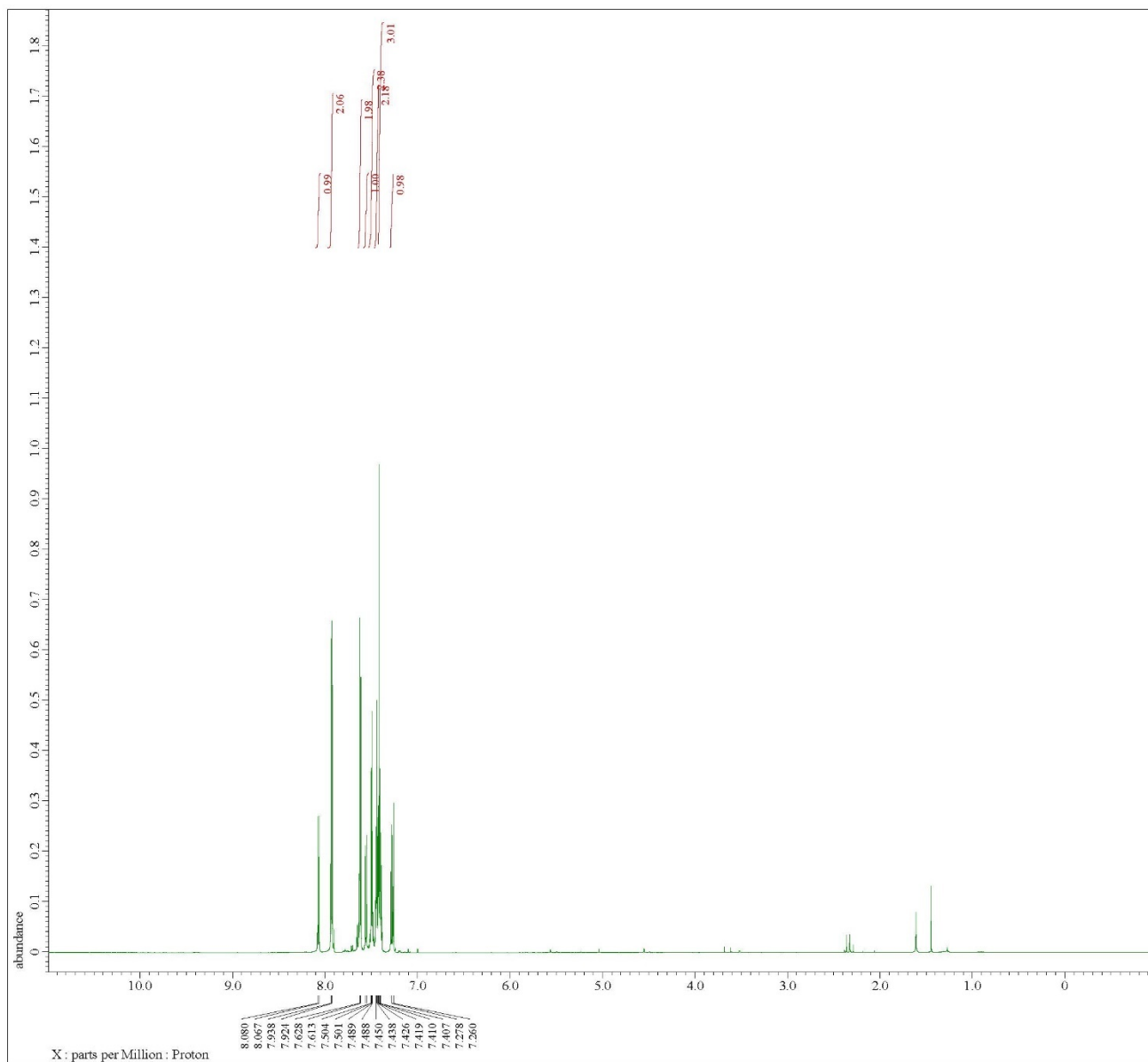
---- PROCESSING PARAMETERS ----
blp.cld(16, 64, 1)
sepf(2.0[Hz], 0.0[s])
ftt(1, TRUE, TRUE)
machephase
ppm

Filename = TK-10-064-1 Mbs_carbon-1-3.jdf
Author = delta
Experiment = carbon13xp
Sample_id = TK-10-064-1 Mbs
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-APR-2025 21:59:14
Revision_Time = 28-APR-2025 22:07:39

Data_Format = 1D COMPLEX
Din_Size = 26214
X_Domain = Carbon13
Din_Title = Carbon13
Din_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/53

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.63206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44456109[Hz]
X_Sweep = 47.34848485[KHz]
X_Sweep_Clipped = 37.87878788[KHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 8[ppm]
Blanking = 15.0[us]
Clipped = FALSE
Scans = 128
Total_Scans = 128

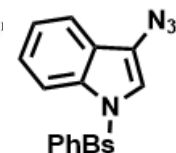
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Gst = 20.6[degC]
X_90_Width = 8.1[us]
X_Acq_Time = 0.63206016[s]
X_Angle = 30[deg]
X_Atn = 11[db]
X_Pulse = 2.7[us]
Irr_Atn_Dec = 25.803[db]
Irr_Atn_Dec_Calc = 25.803[db]
Irr_Atn_Dec_Default_Calc = 25.803[db]
Irr_Atn_Noise = 25.803[db]
Irr_Dec_Bandwidth_Hz = 7.23684211[KHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_DecCoupling = TRUE
Irr_Noise = TRUE
Irr_Noise = VAL72
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 = 2[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 2.63206016[s]



```

---- PROCESSING PARAMETERS ----
sext( 0.2[Hz], 0.0[F] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinphase
ppm

```



4e

```

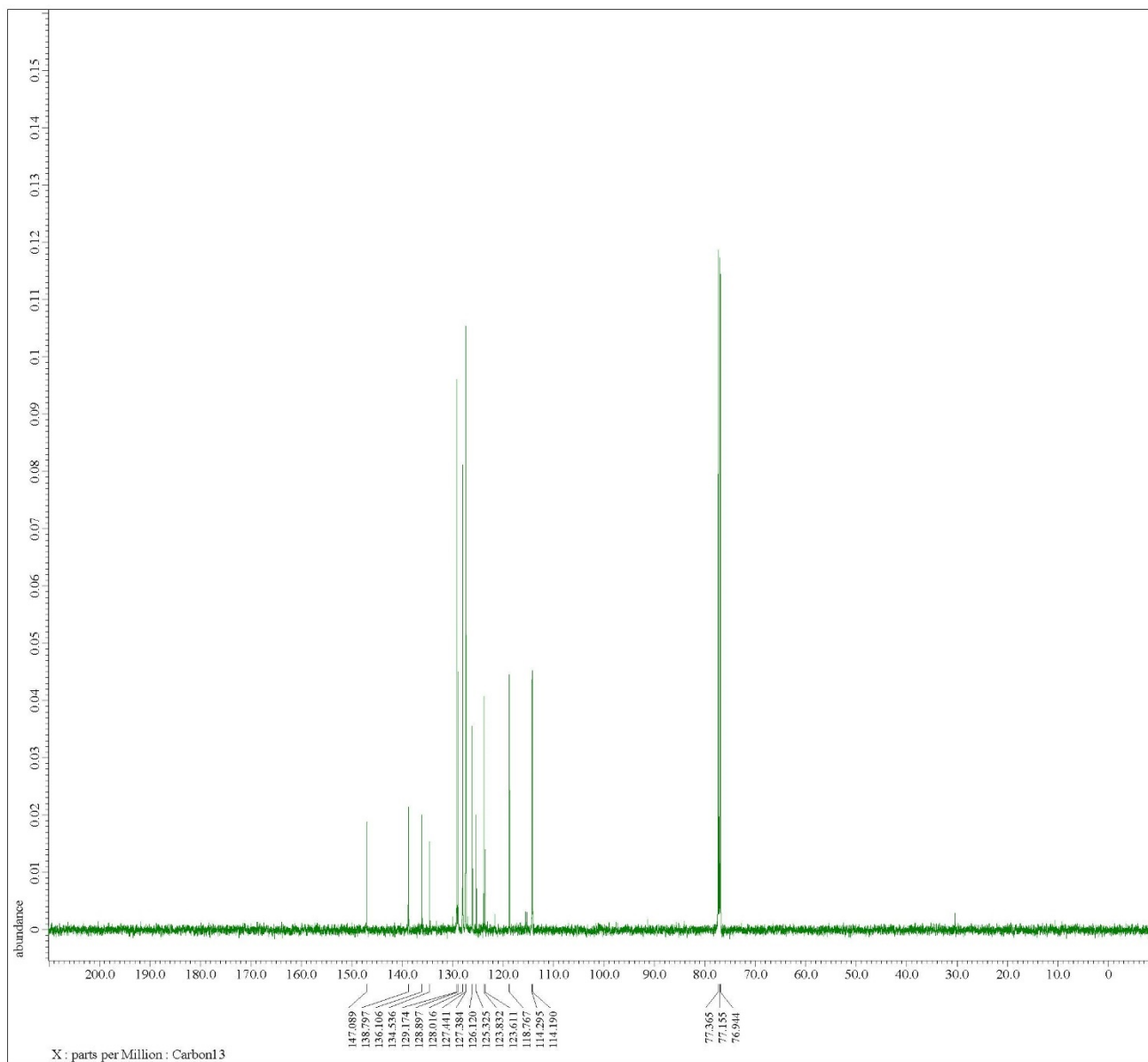
Filename      = TK-10-065-1 PhBs_proton-1-3.jdf
Author        = delta
Experiment    = proton_1xp
Sample_id     = TK-10-065-1 PhBs
Solvent       = CHLOROFORM-D
Actual_Start_Time = 29-APR-2025 20:36:21
Revision_Time = 30-APR-2025 10:10:38

Data_Format   = 1D COMPLEX
Dim_Size      = 36214
X_Domain      = Proton
Dim_Title     = Proton
Dim_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ600R/S3

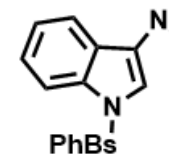
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.90455552[s]
X_Domain      = Proton
X_Freq        = 600.1723046[MHz]
X_Offset      = 5[ppm]
X_Points      = 32768
X_Prescans    = 1
X_Resolution  = 0.34428676[Hz]
X_Sweep       = 11.28158845[kHz]
X_Sweep_Clipped = 9.02527076[kHz]
f1c_Domain    = Proton
f1c_Freq      = 600.1723046[MHz]
f1c_Offset    = 5[ppm]
f2c_Domain    = Proton
f2c_Freq      = 600.1723046[MHz]
f2c_Offset    = 5[ppm]
Blanking      = 5.0[us]
Clipped       = FALSE
Scans         = 4
Total_Scans   = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 36
Temp_Set        = 19.9[degC]
X_90_Width      = 10.5[us]
X_Acq_Time      = 2.90455552[s]
X_Angle         = 45[deg]
X_Attn          = 8.1[dB]
X_Pulse         = 6.25[us]
TEC_Mode        = Off
TE1_Mode        = Off
Dante_Loop      = 200
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase           = {0, 90, 270, 180, 180, 270, 90, 0}
Preset_Time     = 2[s]
Preset_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)
 sepf(2.0[MHz], 0.0[s])
 ftc(1, TRUE, TRUE)
 machinephase
 ppm



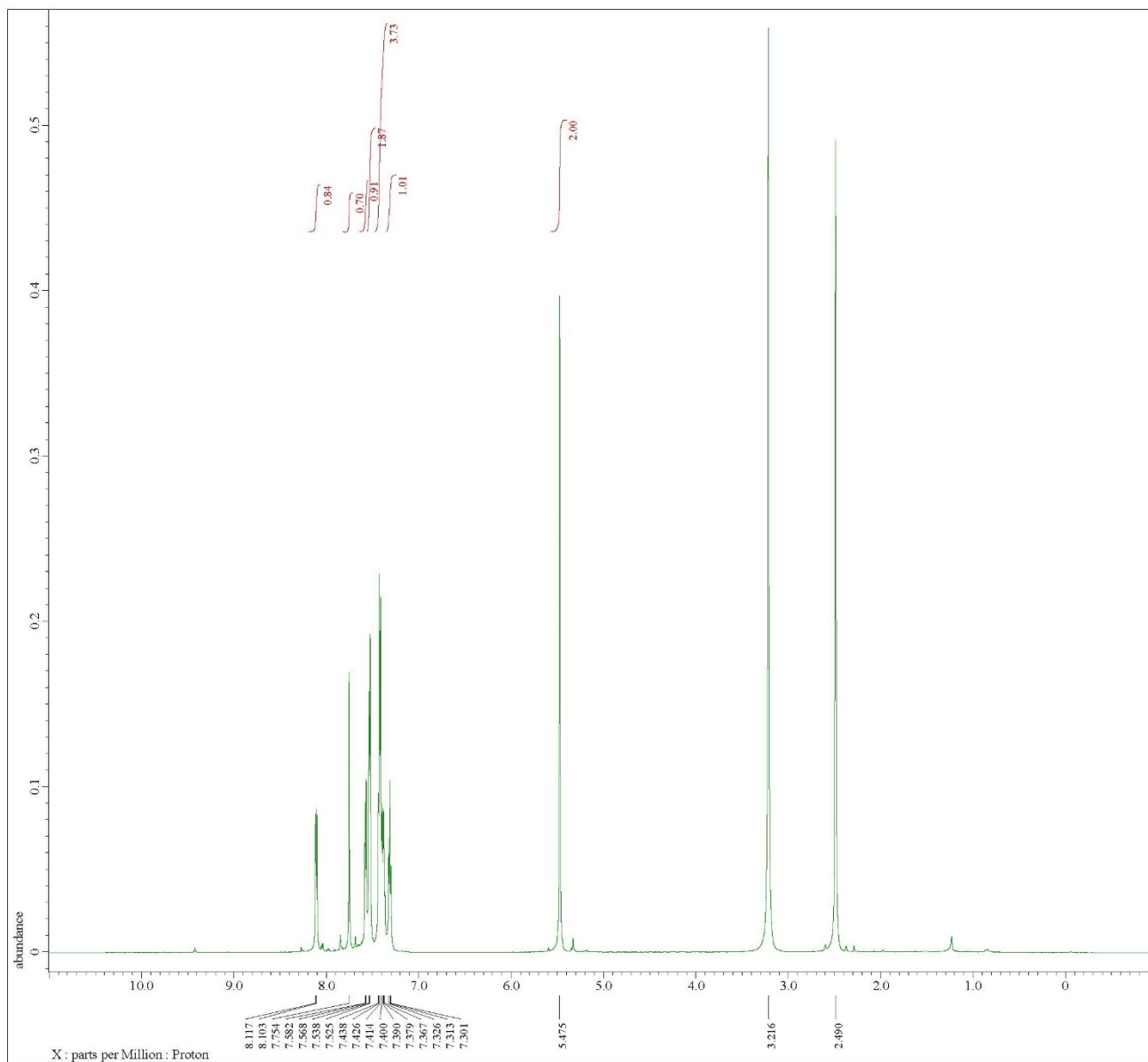
4e

Filename = TX-10-065-1 PhBs_carbon-1-2.jdf
 Author = Delta
 Experiment = carbon-13p
 Sample_id = TX-10-065-1 PhBs
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 29-APR-2025 20:37:23
 Revision_Time = 29-APR-2025 22:35:45

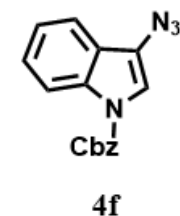
Data_Format = 1D COMPLEX
 Bin_Size = 26214
 X_Domain = Carbon13
 Bin_Title = Carbon13
 Bin_Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ600R/53

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 = 1.44493109[Hz]
 X_Sweep = 47.34848485[kHz]
 X_Sweep_Clipped = 37.87878788[kHz]
 Irc_Domain = proton
 Irc_Freq = 600.1723046[MHz]
 Irc_Offset = 5[ppm]
 Blanking = 15.0[us]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 16

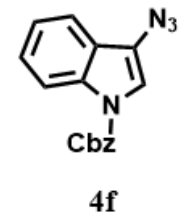
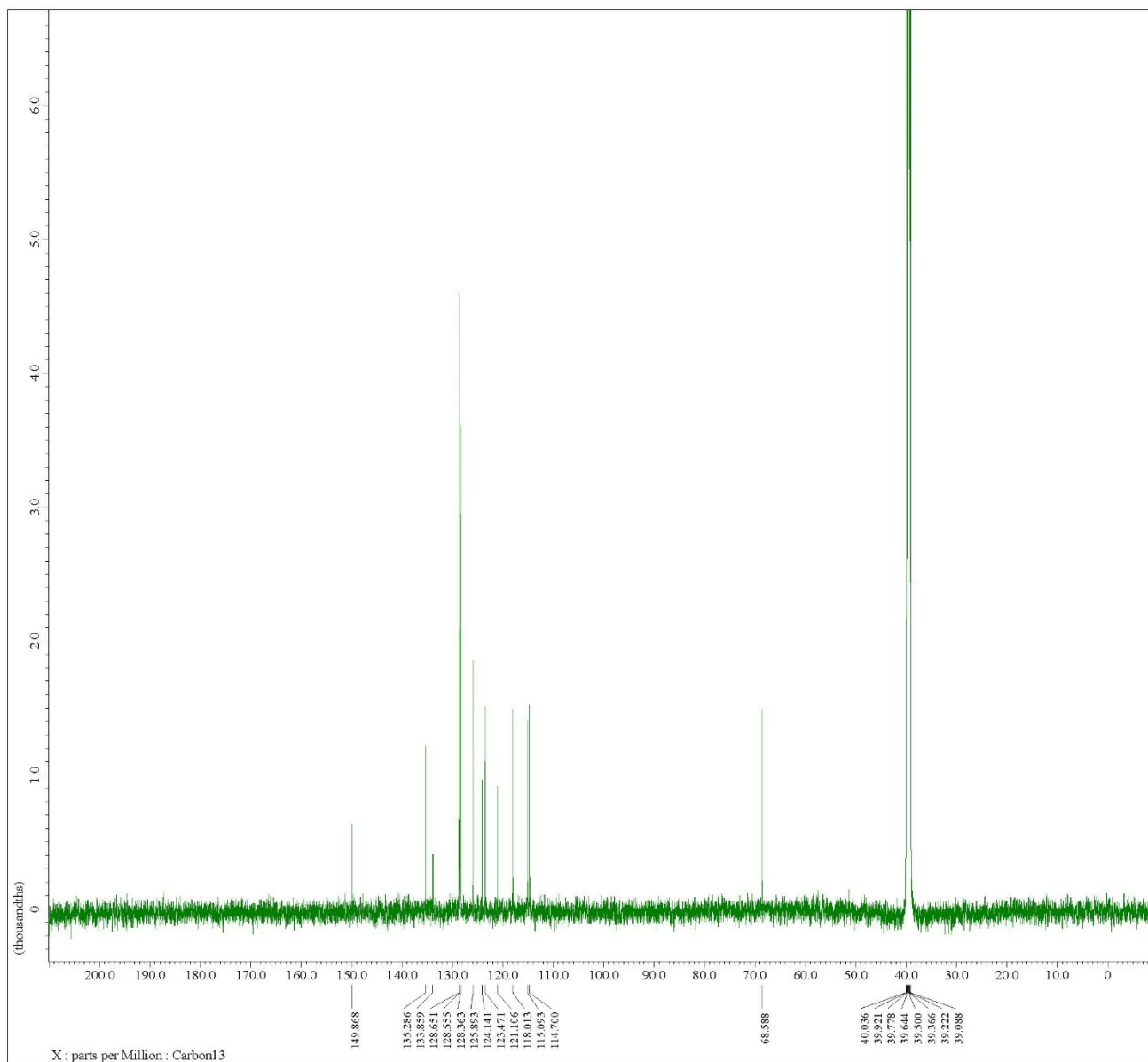
Relaxation_Delay = 2[s]
 Recvr_Gain = 56
 Temp_Get = 19.9[deg]
 X_90_Width = 8.1[us]
 X_Acq_Time = 0.69206016[s]
 X_Angle = 30[deg]
 X_Atn = 11[db]
 X_Pulse = 2.7[us]
 Irc_Atn_Dec = 25.803[db]
 Irc_Atn_Dec_Calc = 25.803[db]
 Irc_Atn_Dec_Default_Calc = 25.803[db]
 Irc_Atn_Noise = 25.803[db]
 Irc_Dec_Bandwidth_Hz = 7.23684211[kHz]
 Irc_Dec_Bandwidth_Ppm = 12.05794078[ppm]
 Irc_Dec_Freq = 600.1723046[MHz]
 Irc_Dec_Merit_Factor = 2.2
 Irc_Decoupling = TRUE
 Irc_Noise = TRUE
 Irc_Noise = VAL77
 Irc_Offset_Default = 5[ppm]
 Irc_Pwidth = 76[us]
 Irc_Pwidth_Default = 76[us]
 Irc_Pwidth_Default_Calc = 76[us]
 Irc_Pwidth_Templ = 76[us]
 Irc_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 -----
 blip_cld(16, 64, 1)
 sepf(2.0[Hz], 0.0[s])
 ftc(1, TRUE, TRUE)
 machinephase
 ppm



Filename = SR-2-039-crude-2 DMSO_proton-2-3.jdf
 Author = delta
 Experiment = proton_1xp
 Sample_id = SR-2-039-crude-2 DMSO
 Solvent = DMSO-D6
 Actual_Start_Time = 27-APR-2025 10:40:30
 Revision_Time = 28-APR-2025 23:17:06
 Data_Format = 1D_COMPLEX
 Bin_Size = 36214
 X_Domain = Proton
 Bin_Title = Proton
 Bin_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]
 Ict_Domain = Proton
 Ict_Freq = 600.1723046[MHz]
 Ict_Offset = 5[ppm]
 Tel_Domain = Proton
 Tel_Freq = 600.1723046[MHz]
 Tel_Offset = 5[ppm]
 Blanking = 5.0[us]
 Clipped = FALSE
 Scans = 8
 Total_Scans = 8
 Relaxation_Delay = 2[s]
 Recvr_Gain = 56
 Temp_Set = 50[deg]
 X_90_Width = 10.5[us]
 X_Acq_Time = 2.90455552[s]
 X_Angle = 45[deg]
 X_Atn = 8.1[db]
 X_Pulse = 6.25[us]
 Tfr_Mode = off
 Tel_Mode = off
 Dntr_Loop = 200
 Dntr_Preset = 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]



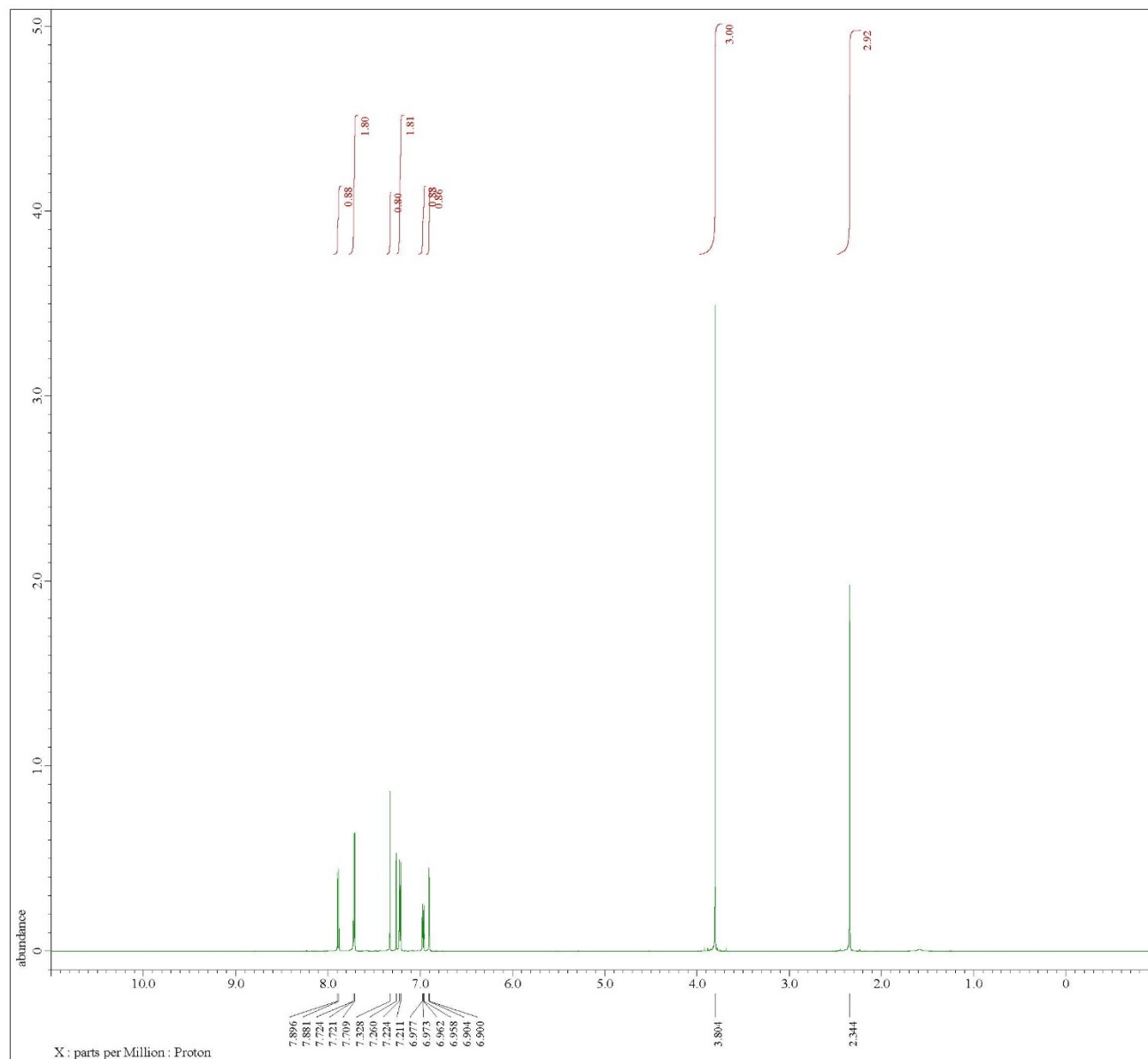
----- PROCESSING PARAMETERS -----
blp.cld(16, 64, 1)
sepf(2.0[MHz], 0.0[s])
fft(1, TRUE, TRUE)
machephase
ppm

Filename = SA-2-039-crude2_carbon-1-2.jdf
Author = delta
Experiment = carbon-13p
Sample_id = SA-2-039-crude2
Solvent = DMSO-d6
Actual_Start_Time = 28-APR-2025 22:14:30
Revision_Time = 28-APR-2025 22:51:41

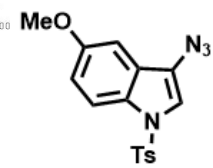
Data_Format = 1D_COMPLEX
Din_Size = 26214
X_Domain = Carbon13
Din_Title = Carbon13
Din_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/53

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.63206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44456109[Hz]
X_Sweep = 47.34848485[KHz]
X_Sweep_Clipped = 37.87878788[KHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 8[ppm]
Blanking = 15.0[us]
Clipped = TRUE
Scans = 800
Total_Scans = 800

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Gst = 20[deg]
X_90_Width = 8.1[us]
X_Acq_Time = 0.63206016[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_Noise = 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 = 2.3
Irr_Decoupling = TRUE
Irr_Noise = TRUE
Irr_Noise = VAL72
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 = 2[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 2.63206016[s]



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

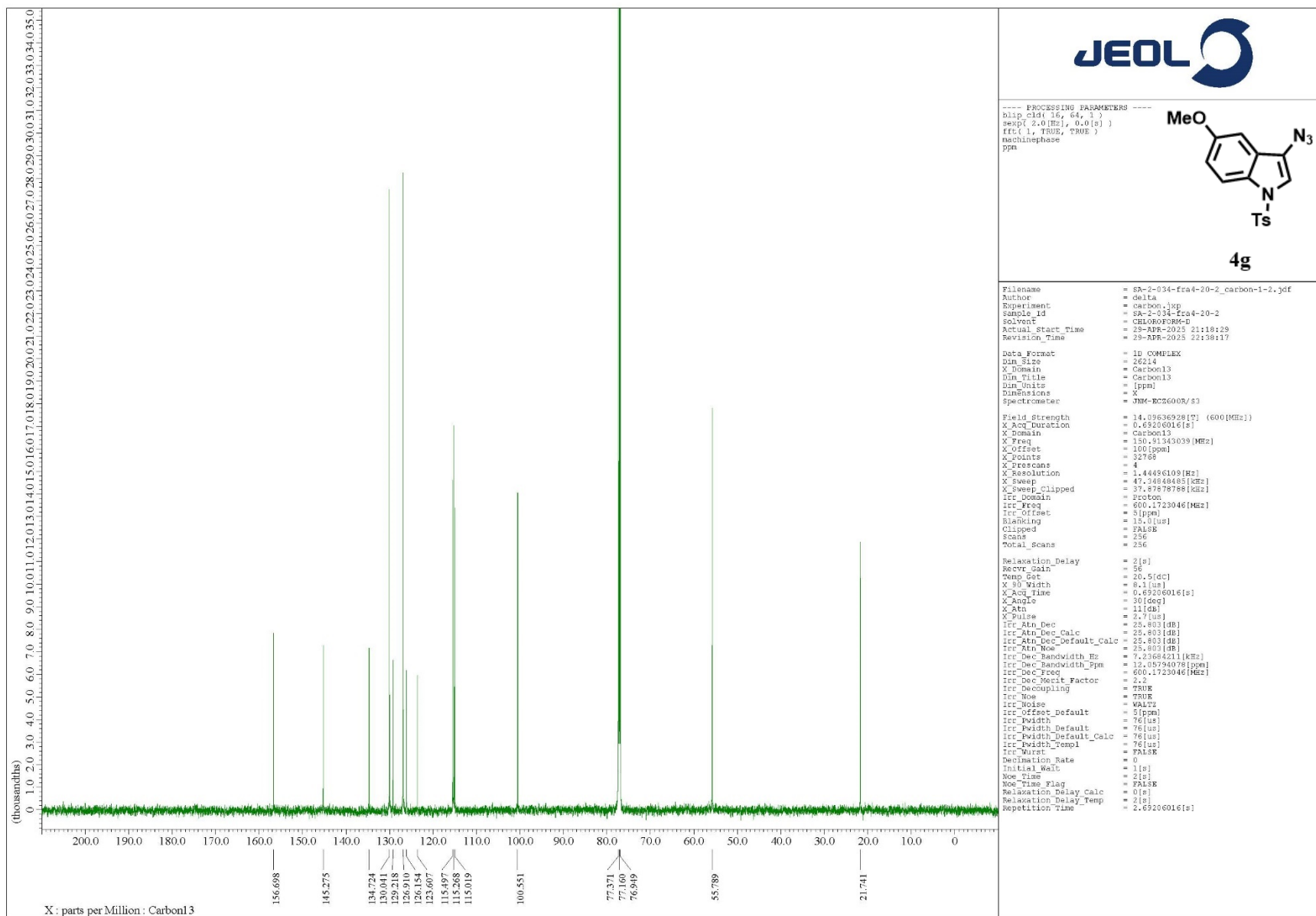


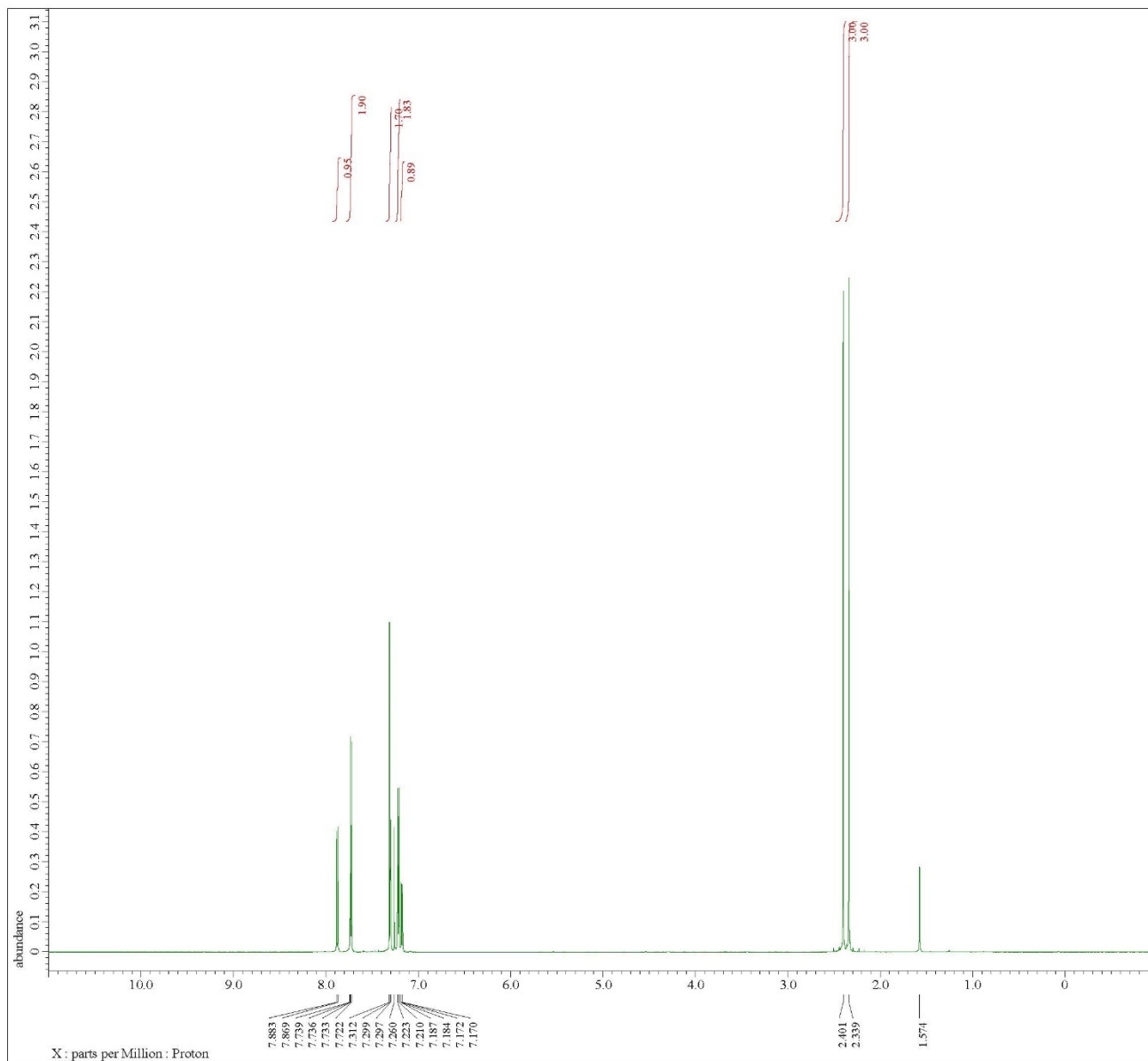
Filename = SA-2-034-fra4-20-2_proton-1-3.jdf
 Author = delta
 Experiment = proton.mxp
 Sample_id = SA-2-034-fra4-20-2
 solvent = CHLOROFORM-D
 Actual_Start_Time = 29-APR-2025 20:06:14
 Revision_Time = 30-APR-2025 10:45:51

Data_Format = 1D COMPLEX
 Din_Size = 26214
 X_Domain = Proton
 Din_Title = Proton
 Din_Units = [ppm]
 Dimensions = 1
 Spectrometer = JNM-ECZ600R/S3

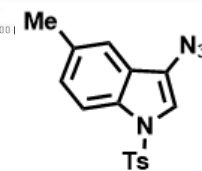
Field_Strength = 14.09636928[T] (600[MHz])
 X_Acq_Duration = 2.90455552[s]
 X_Domain = Proton
 X_Freq = 600.1723046[MHz]
 X_Offset = 5[ppm]
 X_Points = 32768
 X_Prescans = 1
 X_Resolution = 0.34428676[Hz]
 X_Sweep = 11.28158845[kHz]
 X_Sweep_Clipped = 9.02527076[kHz]
 ITC_Domain = Proton
 ITC_Freq = 600.1723046[MHz]
 ITC_Offset = 5[ppm]
 TCI_Domain = Proton
 TCI_Freq = 600.1723046[MHz]
 TCI_Offset = 5[ppm]
 Blanking = 5.0[us]
 Clipped = FALSE
 Scans = 4
 Total_scans = 4

Relaxation_Delay = 2[s]
 Recvr_Gain = 46
 Temp_Set = 21.1[deg]
 X_90_Width = 10.5[us]
 X_Acq_Time = 2.90455552[s]
 X_Angle = 45[deg]
 X_Atn = 8.1[db]
 X_Pulse = 5.25[us]
 ITC_Mode = off
 TCI_Mode = off
 DanLo_Loop = 200
 Danto_Preset = FALSE
 Decimation_Rate = 0
 Initial_Wait = 1[s]
 Phase = [0, 90, 270, 180, 180, 270, 90, 0]
 Preset_Time = 2[s]
 Preset_Time_Flag = FALSE
 Relaxation_Delay_Calc = 0[s]
 Relaxation_Delay_Temp = 2[s]
 Repetition_Time = 4.90455552[s]



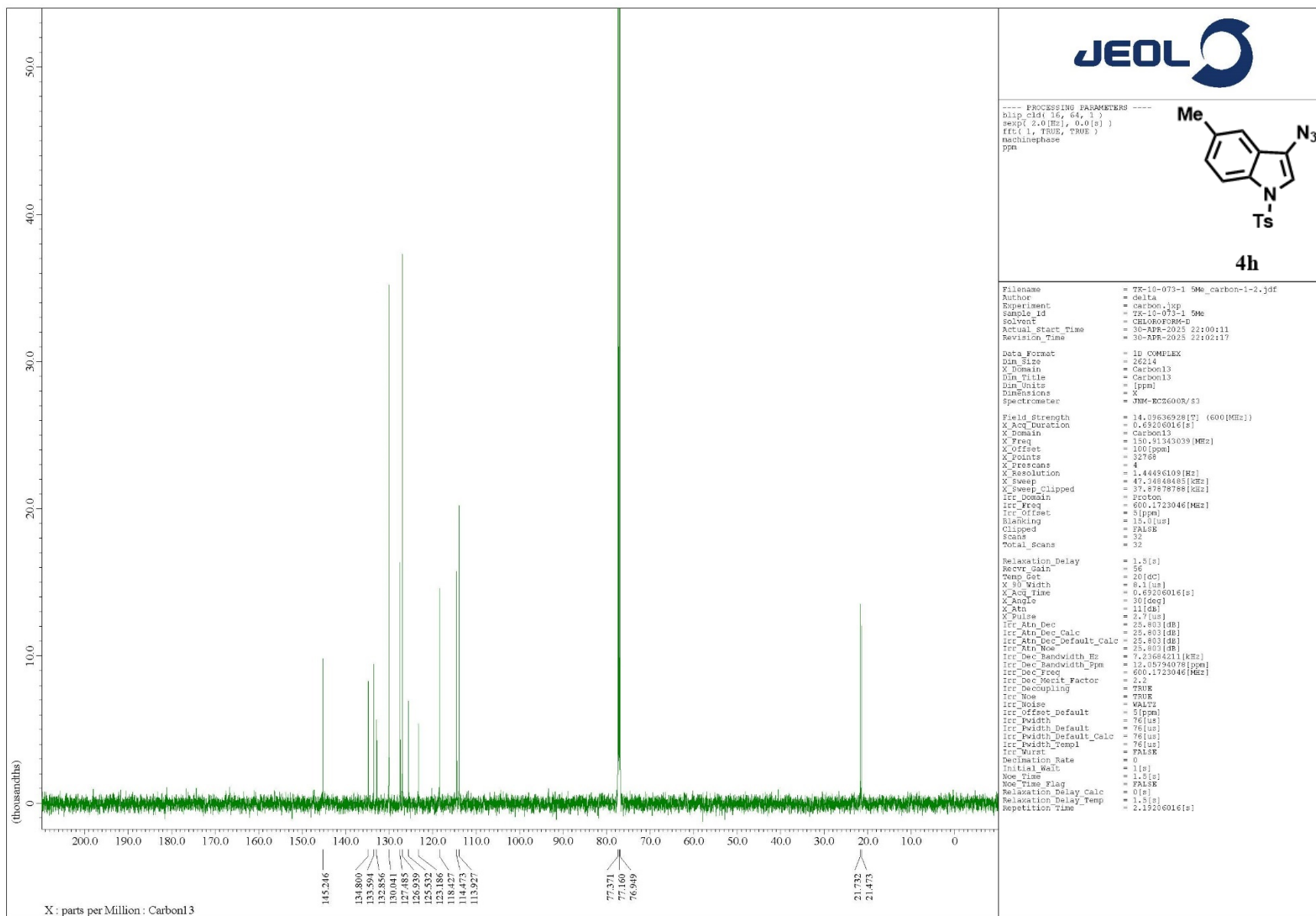


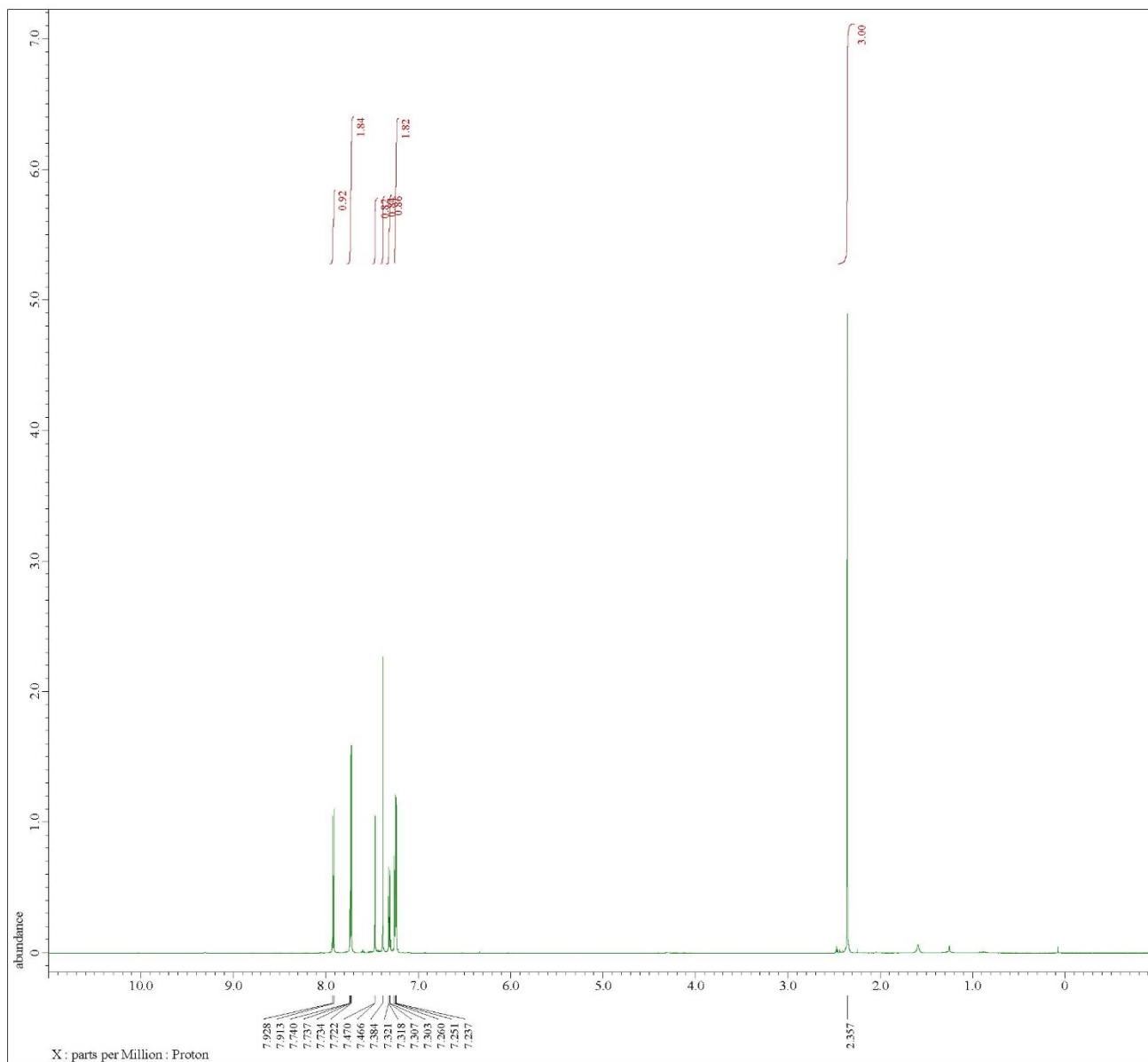
---- PROCESSING PARAMETERS ----
sexpr(0.2[Hz], 0.0[F])
trapezoid(0[Hz], 0[Hz], 80[Hz], 100[Hz])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm



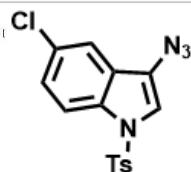
4h

Filename = TK-10-070-1 5Mg_proton-1-3.jdf
Author = delta
Experiment = proton_1xp
Sample_id = TK-10-070-1 5Mg
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-APR-2025 21:58:12
Revision_Time = 1-MAY-2025 08:55:50
Data_Format = 1D_COMPLEX
Bin_Size = 36214
X_Domain = Proton
Bin_Title = Proton
Bin_Units = [ppm]
Dimensions = 1
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 = 0.43849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
F1_Domain = Proton
F1_Freq = 600.1723046[MHz]
F1_Offset = 5[ppm]
F2_Domain = Proton
F2_Freq = 600.1723046[MHz]
F2_Offset = 5[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 2[s]
Recvr_Gain = 46
Temp_Set = 19.9[degC]
X_90_Width = 10.5[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 8.1[dB]
X_Pulse = 8.25[us]
TEC_Mode = Off
TEC_Temp = Off
Dante_Loop = 200
Dante_Preset = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18103808[s]



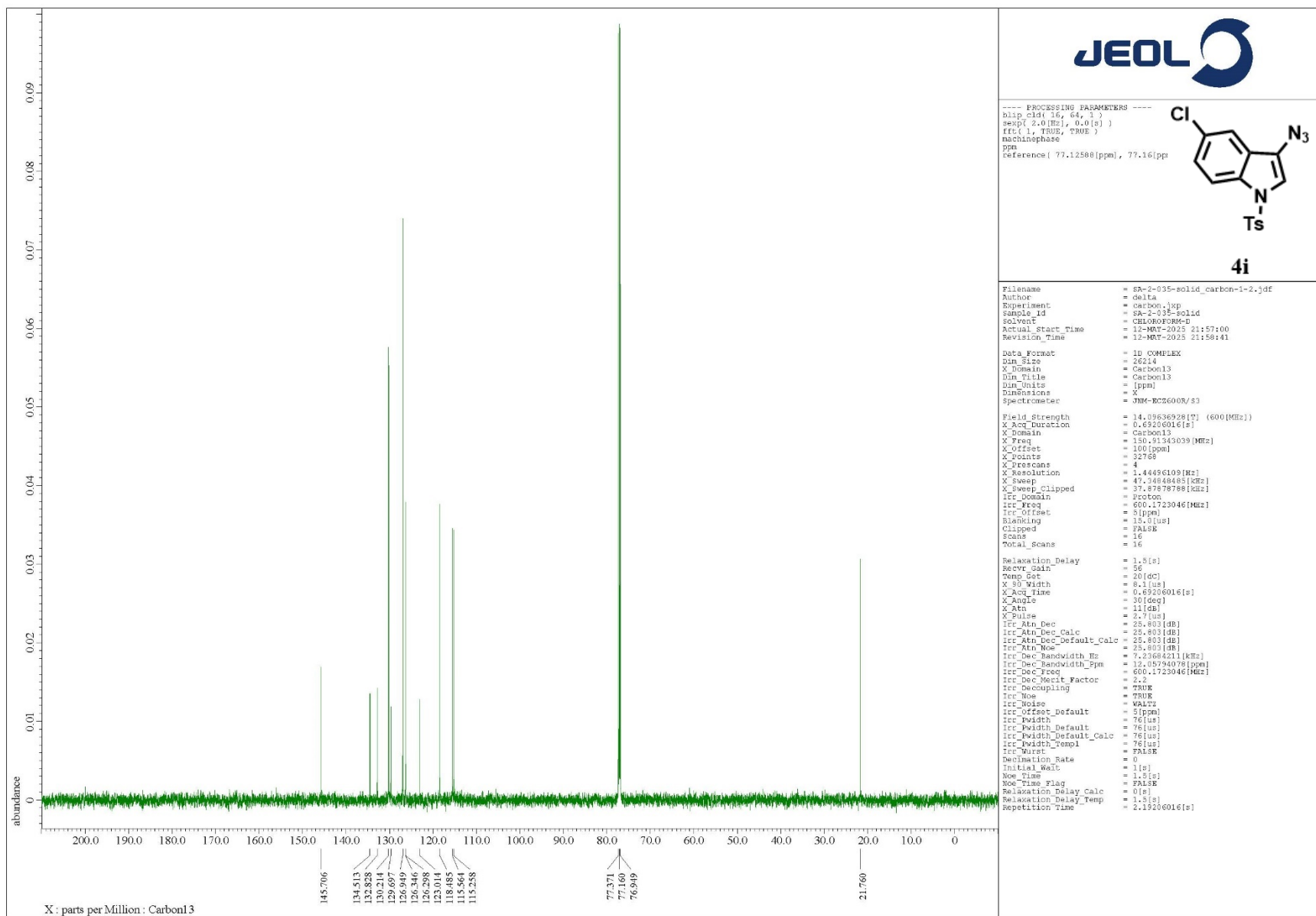


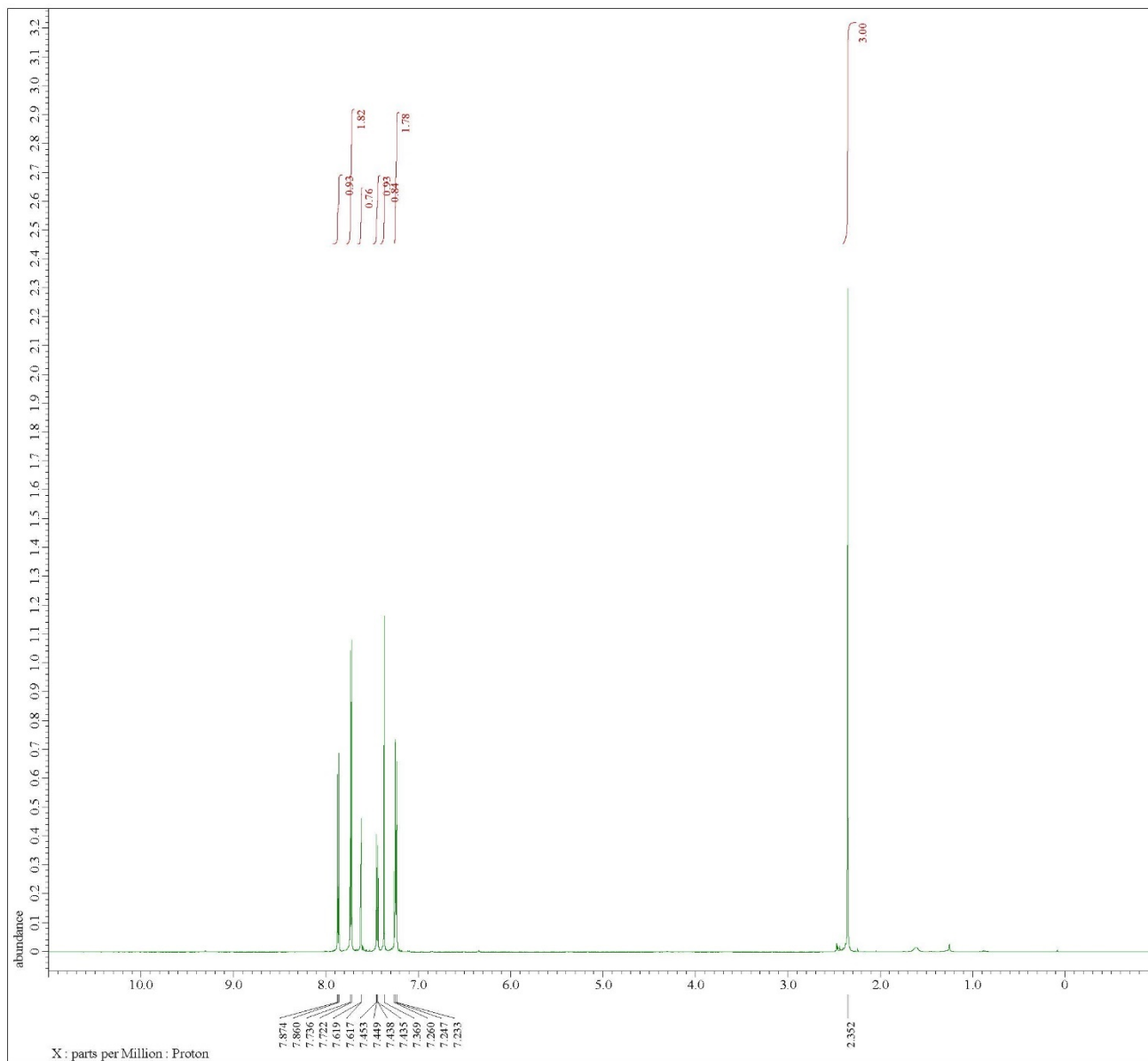
---- PROCESSING PARAMETERS ----
sexpr(0.2[Hz], 0.0[F]
trapezoid(0[%], 0[%], 80[%], 100[
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm



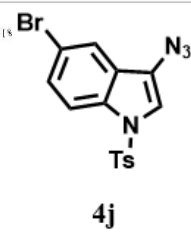
4i

Filename = SR-2-035-solid_proton-1-3.jdf
Author = delta
Experiment = proton_1xp
Sample_id = SR-2-035-solid
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-MAY-2025 21:54:45
Revision_Time = 20-MAY-2025 10:26:27
Data_Format = 1D_COMPLEX
Bin_Size = 36214
X_Domain = Proton
Bin_Title = Proton
Bin_Units = [ppm]
Dimensions = 1
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 = 0.43849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
F1_Domain = Proton
F1_Freq = 600.1723046[MHz]
F1_Offset = 5[ppm]
F2_Domain = Proton
F2_Freq = 600.1723046[MHz]
F2_Offset = 5[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 2[s]
Recvr_Gain = 46
Temp_Set = 20.4[deg]
X_90_Width = 10.5[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 8.1[db]
X_Pulse = 8.25[us]
F1_Mode = Off
F2_Mode = Off
Dante_Loop = 200
Dante_Preset = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18103808[s]

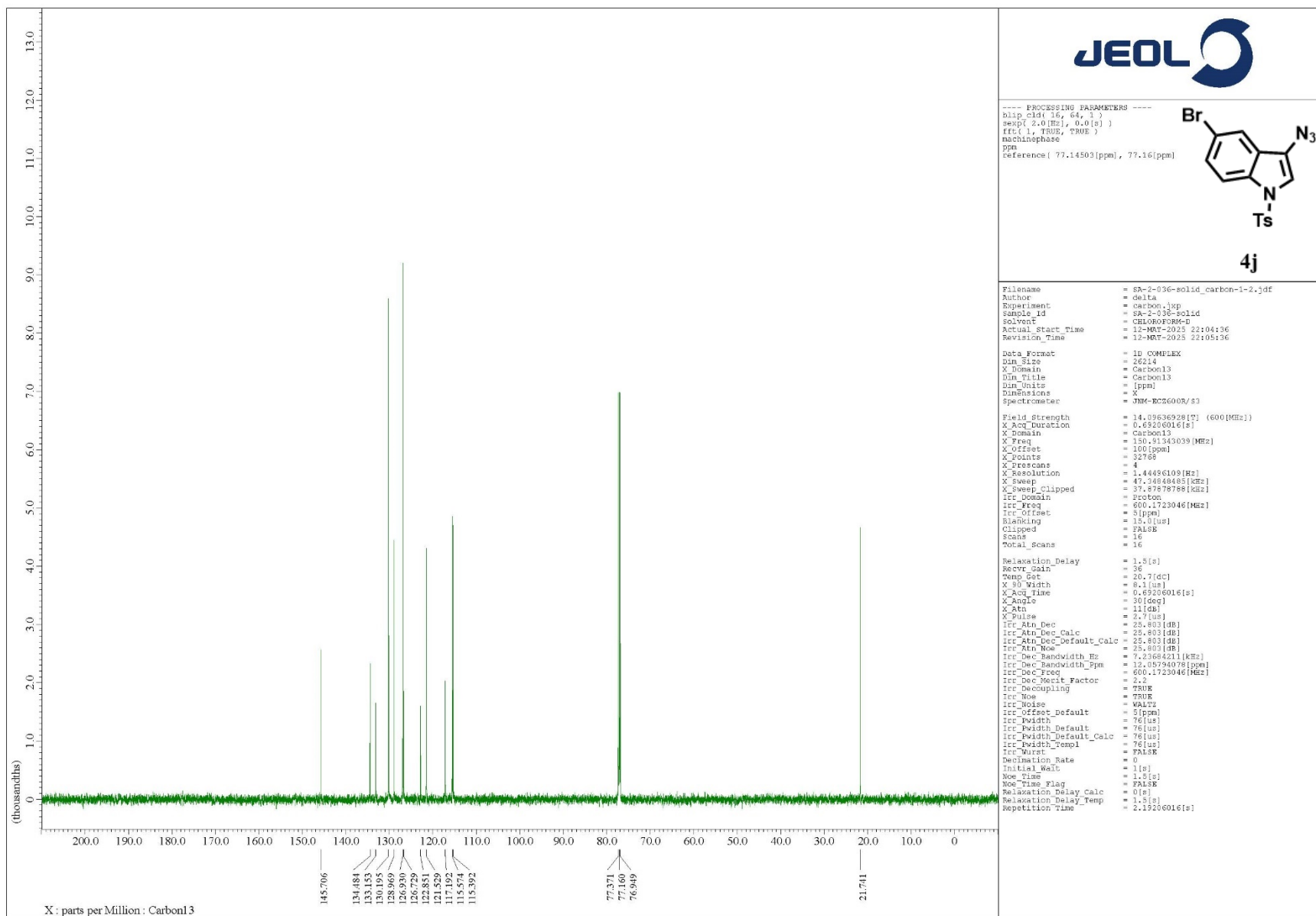


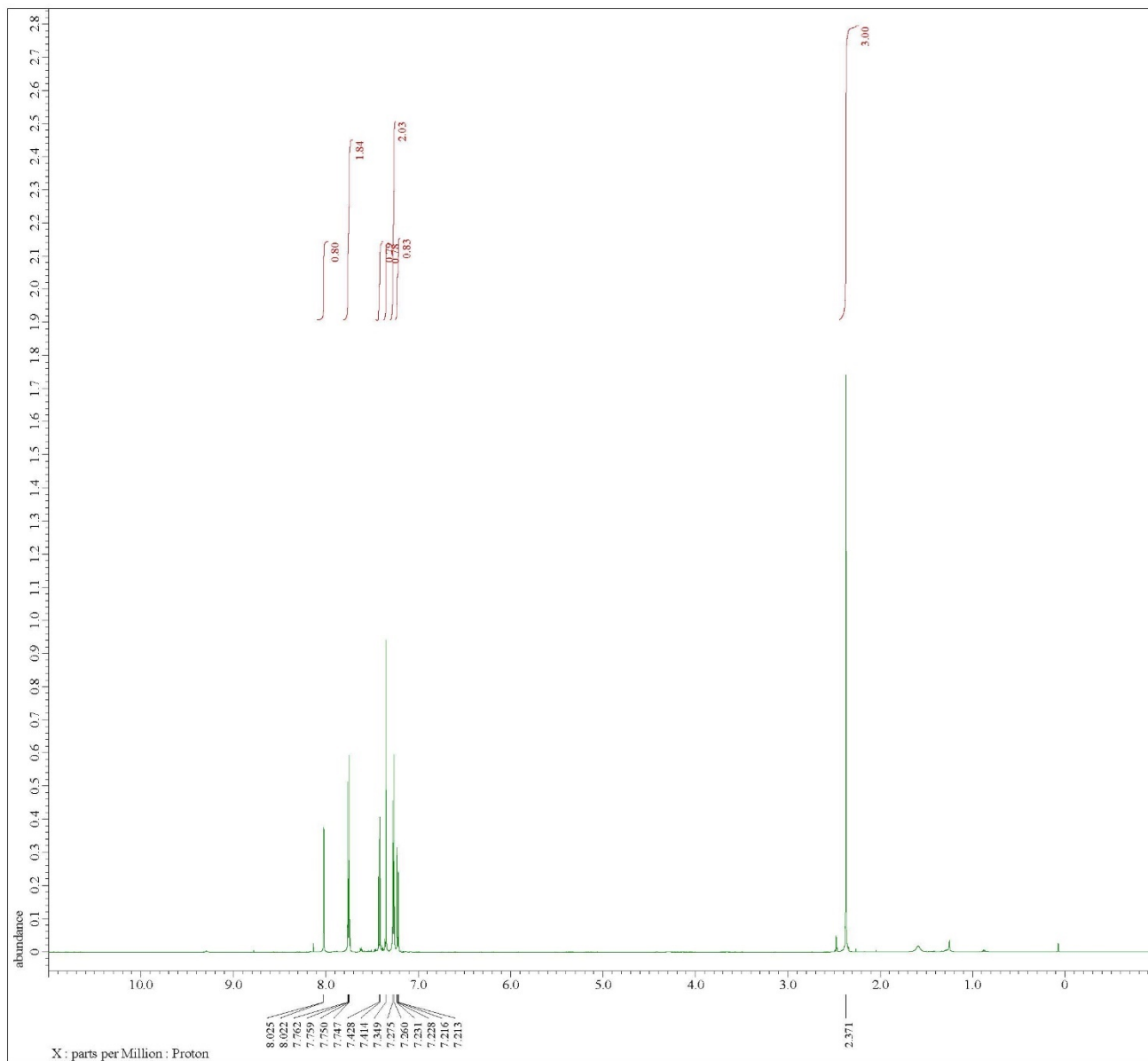


----- PROCESSING PARAMETERS -----
sexpr(0.2[Hz], 0.0[F]
trapezoid(0[%], 0[%], 80[%], 100[%]
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm

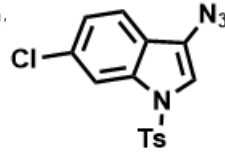


Filename = SR-2-036-solid-2_proton-1-3.jdf
Author = delta
Experiment = proton_1xp
Sample_id = SR-2-036-solid-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-MAY-2025 22:43:38
Revision_Time = 20-MAY-2025 10:24:38
Data_Format = 1D COMPLEX
Data_Size = 26214
X_Domain = Proton
Data_Title = Proton
Data_Units = [ppm]
Dimensions = 1
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 = 0.43849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
F1_Domain = Proton
F1_Freq = 600.1723046[MHz]
F1_Offset = 5[ppm]
F2_Domain = Proton
F2_Freq = 600.1723046[MHz]
F2_Offset = 5[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 2[s]
Recv_Gain = 36
Temp_Set = 19.9[degC]
X_90_Width = 10.5[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 8.1[db]
X_Pulse = 8.25[us]
TEC_Mode = Off
TEC_Mode = Off
Dante_Loop = 200
Dante_Preset = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18103808[s]



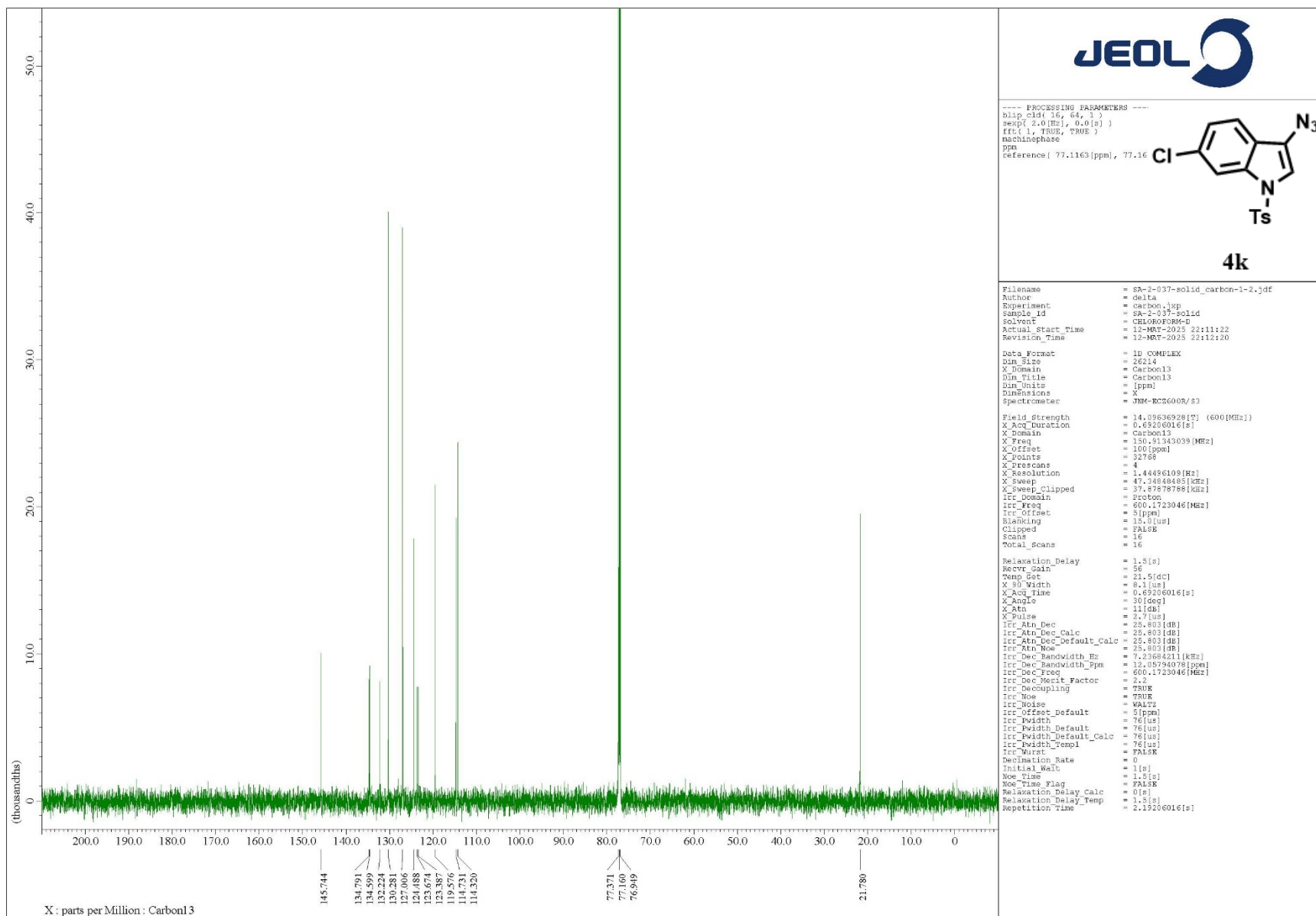


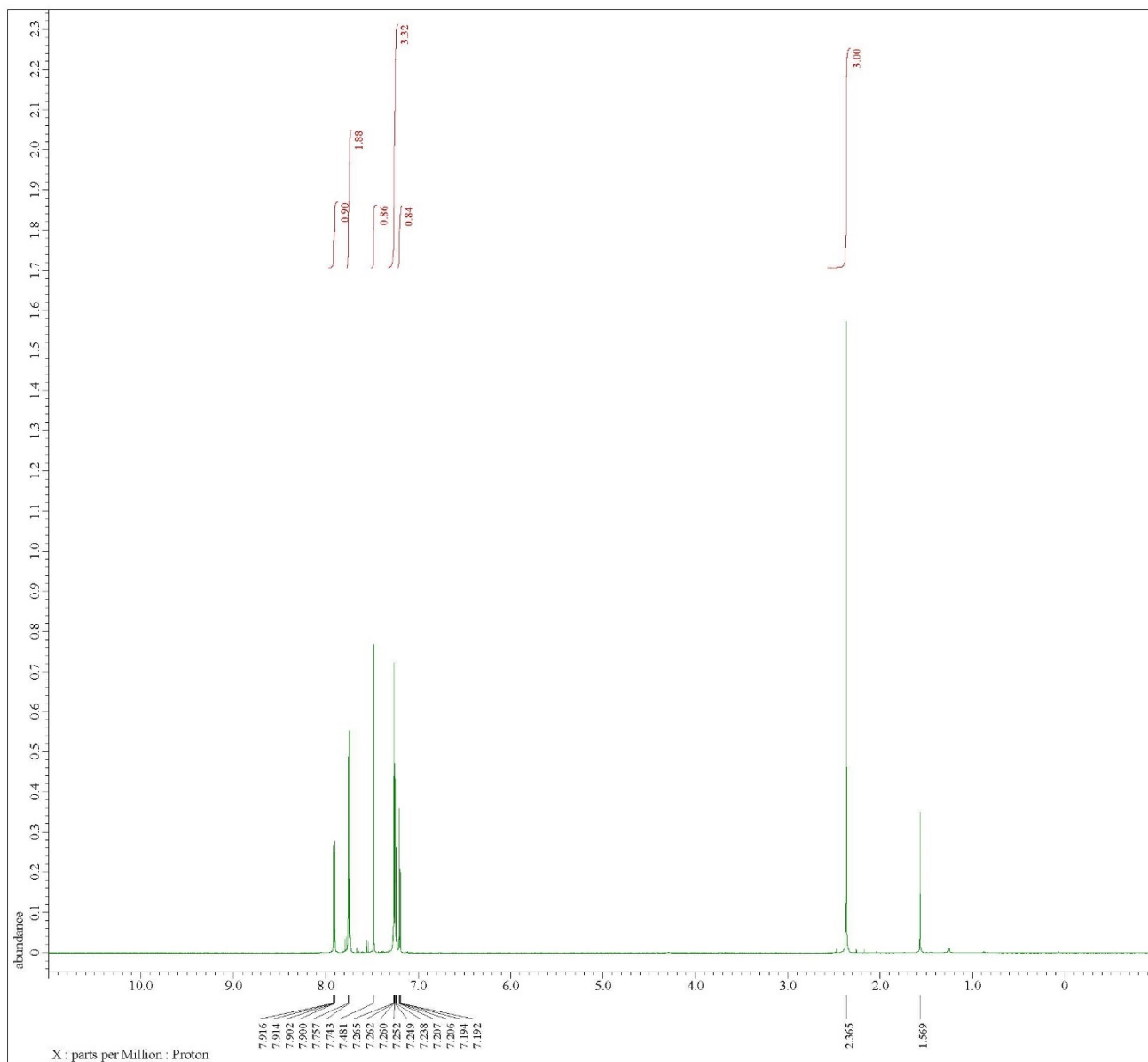
--- PROCESSING PARAMETERS ---
 smpc(0.2[Hz], 0.0[F])
 trapezoid(0[%], 0[%], 80[%],
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm



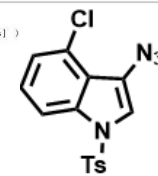
4k

Filename = SR-2-037-solid_proton-1-3.jdf
 Author = delta
 Experiment = proton_1xp
 Sample_id = SR-2-037-solid
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 12-MAY-2025 22:09:09
 Revision_Time = 20-MAY-2025 10:37:43
 Data_Format = 1D_COMPLEX
 Bin_Size = 36214
 X_Domain = Proton
 Din_Title = Proton
 Din_Units = [ppm]
 Dimensions = 1
 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 = 0.43849727[Hz]
 X_Sweep = 15.02403846[kHz]
 X_Sweep_Clipped = 12.01923077[kHz]
 Ict_Domain = Proton
 Ict_Freq = 600.1723046[MHz]
 Ict_Offset = 5[ppm]
 Tel_Domain = Proton
 Tel_Freq = 600.1723046[MHz]
 Tel_Offset = 5[ppm]
 Blanking = 5.0[us]
 Clipped = FALSE
 Scans = 4
 Total_Scans = 4
 Relaxation_Delay = 2[s]
 Recvr_Gain = 36
 Temp_Set = 21.3[degC]
 X_90_Width = 10.5[us]
 X_Acq_Time = 2.18103808[s]
 X_Angle = 45[deg]
 X_Atn = 8.1[db]
 X_Pulse = 6.25[us]
 Tfr_Mode = off
 Tel_Mode = off
 Datto_Leap = 200
 Datto_Preset = 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]





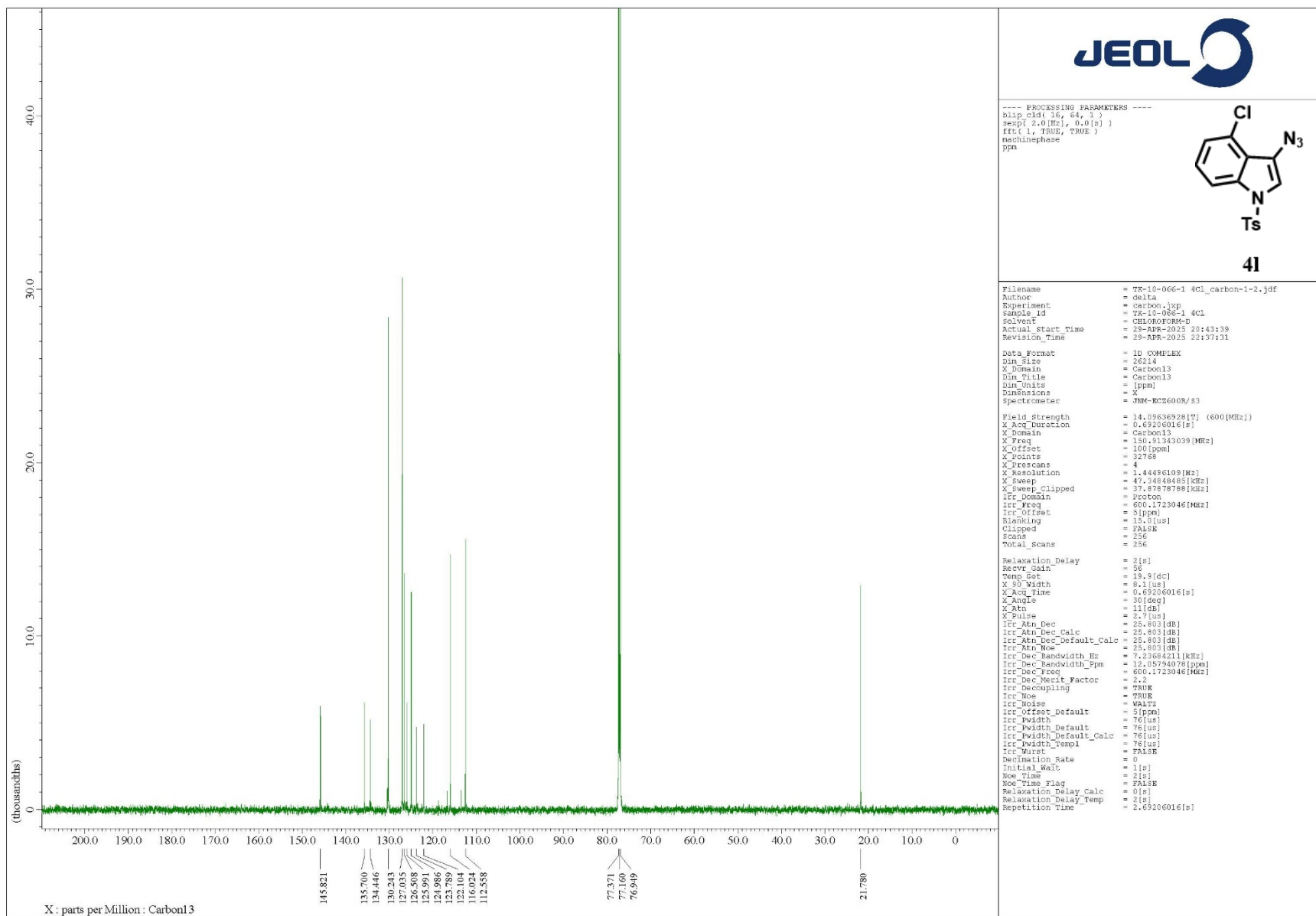
JEOL

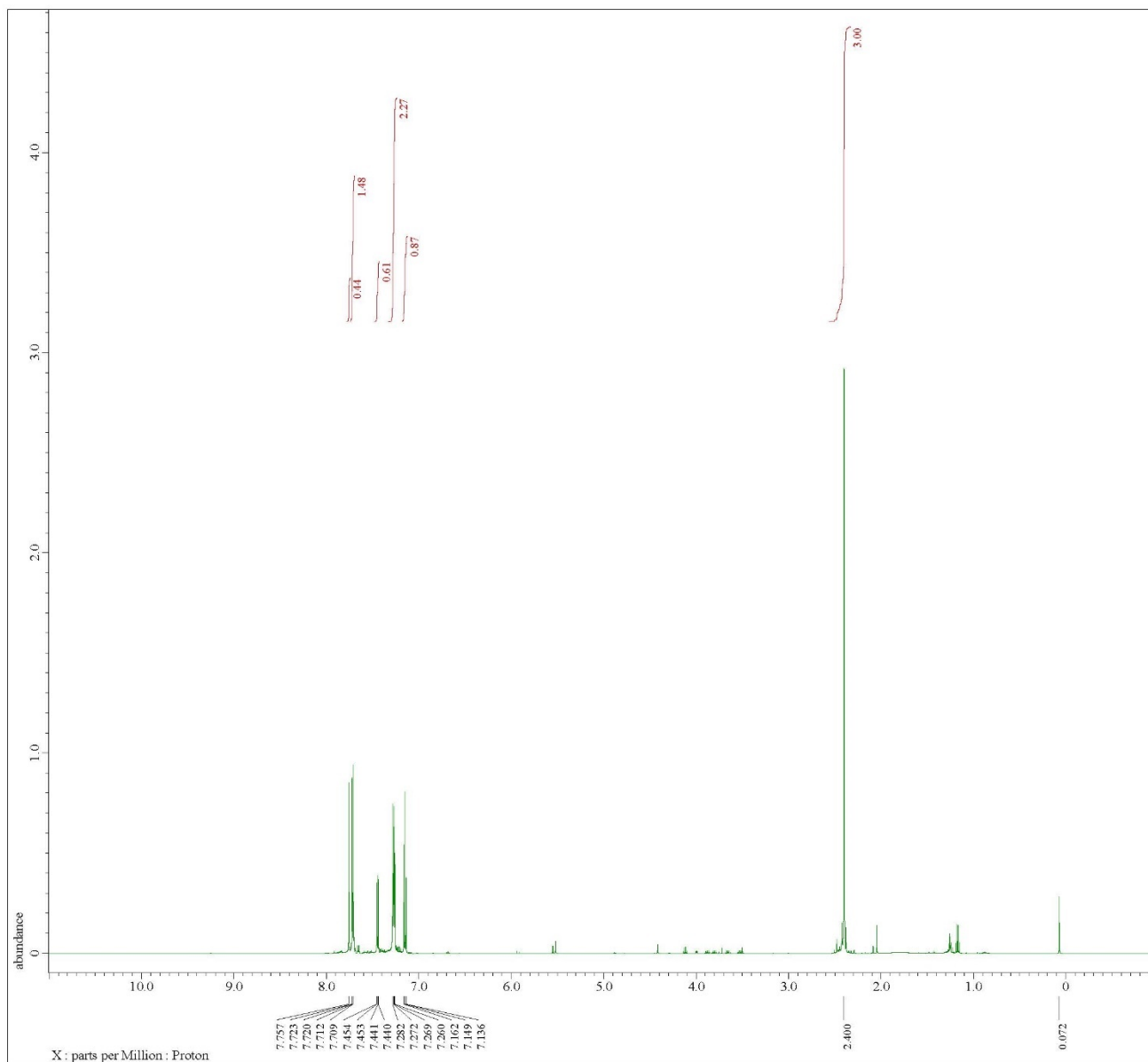


4l

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

Filename = TK-10-066-1 4Cl_proton-1-3.jdf
Author = delta
Experiment = proton_1xp
Sample_id = TK-10-066-1 4cl
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-APR-2025 20:42:36
Revision_Time = 30-APR-2025 10:03:33
Data_Format = 1D_COMPLEX
Bin_Size = 36214
X_Domain = Proton
Bin_Title = Proton
Bin_Units = [ppm]
Dimensions = 1
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_Clippped = 9.02527076[kHz]
Ict_Domain = Proton
Ict_Freq = 600.1723046[MHz]
Ict_Offset = 5[ppm]
Tel_Domain = Proton
Tel_Freq = 600.1723046[MHz]
Tel_Offset = 5[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 2[s]
Recvr_Gain = 46
Temp_Set = 19.9[degC]
X_90_Width = 10.5[us]
X_Acq_Time = 2.90455552[s]
X_Angle = 45[deg]
X_Attn = 8.1[dB]
X_Pulse = 8.25[us]
Tfz_Mode = Off
Tel_Mode = Off
Dante_Loop = 200
Dante_Preset = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.90455552[s]



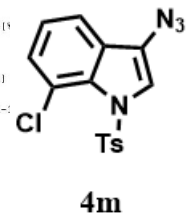


```

---- PROCESSING PARAMETERS ----
sext( 0.2[Hz], 0.0[Hz] )
trapezoid( 0[Hz], 0[Hz], 80[Hz], 100[Hz]
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.24812[ppm], 7.26[ppm]
thresh( 8.43981[Hz], 1, )

```

以下に由来: SA-2-040-fra5-10 proton-1



```

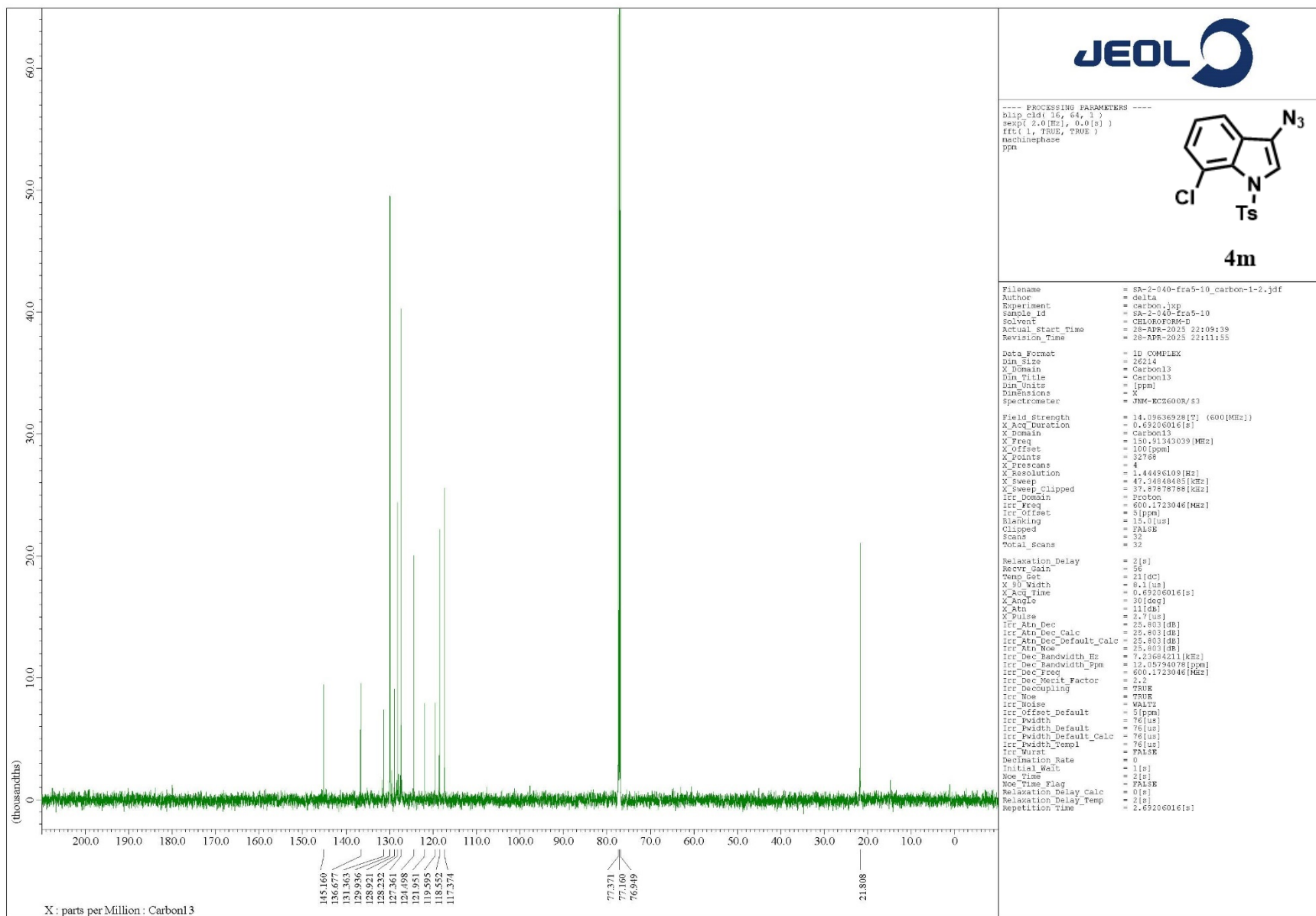
Filename      = SA-2-040-fra5-10_proton-1-2.jdf
Author        = delta
Experiment     = proton.mxp
Sample_id      = SA-2-040-fra5-10
Solvent        = CHLOROFORM-D
Actual_Start_Time = 28-APR-2025 21:17:49
Revision_Time  = 28-APR-2025 23:24:02

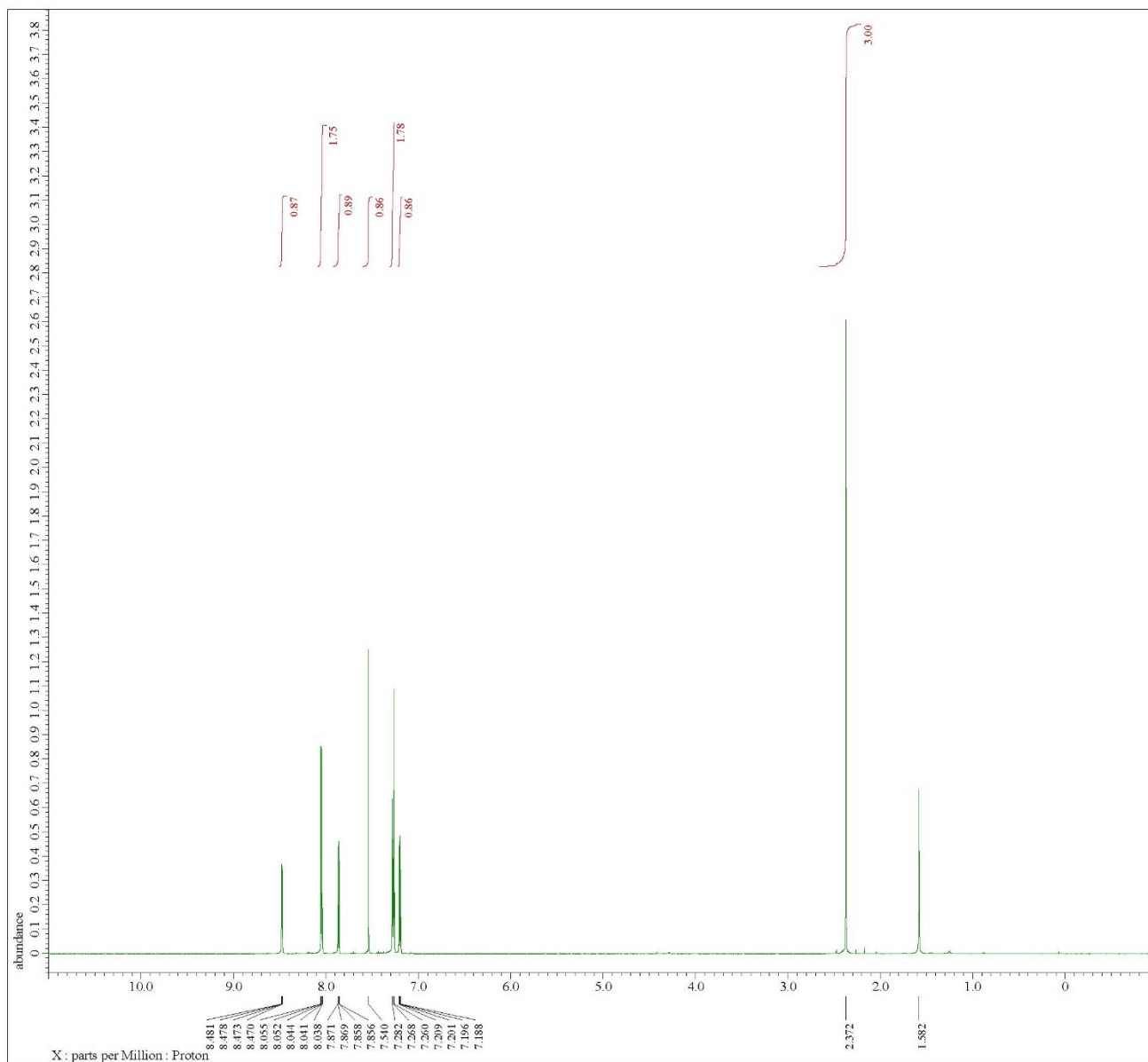
Data_Format    = 1D COMPLEX
Dm_Slice       = 26214
X_Domain       = Proton
Dm_Title       = Proton
Dm_Units       = [ppm]
Dimensions     = X
Spectrometer   = JNM-ECZ600R/S3

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.90455552[s]
X_Domain       = Proton
X_Freq         = 600.1723046[MHz]
X_Offset       = 8[ppm]
X_Points       = 32768
X_Prescans     = 1
X_Resolution   = 0.34428676[Hz]
X_Sweep        = 11.28158845[kHz]
X_Sweep_Clipped = 9.02527076[kHz]
F1_Freq        = 600.1723046[MHz]
F1_Offset      = 8[ppm]
F1_Domain      = Proton
F1_Freq        = 600.1723046[MHz]
F1_Offset      = 8[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_Scans    = 4

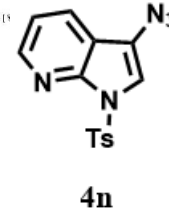
Relaxation_Delay = 2[s]
Recvr_Gain       = 46
Temp_Set         = 20[degC]
X_90_Width       = 10.5[us]
X_Acq_Time       = 2.90455552[s]
X_Angle          = 45[deg]
X_Atn           = 8.1[deg]
X_Pulse          = 8.25[us]
F1_Mode         = off
F1_Node         = off
Dante_Loop       = 200
Dante_Preset     = FALSE
Decimation_Rate  = 0
Initial_Wait     = 1[s]
Phase           = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time      = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time  = 4.90455552[s]

```





---- PROCESSING PARAMETERS ----
 sepr(0.2[Hz], 0.0[Hz])
 trapezoid(0[Hz], 0[Hz], 80[Hz], 100[Hz])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinphase
 ppm

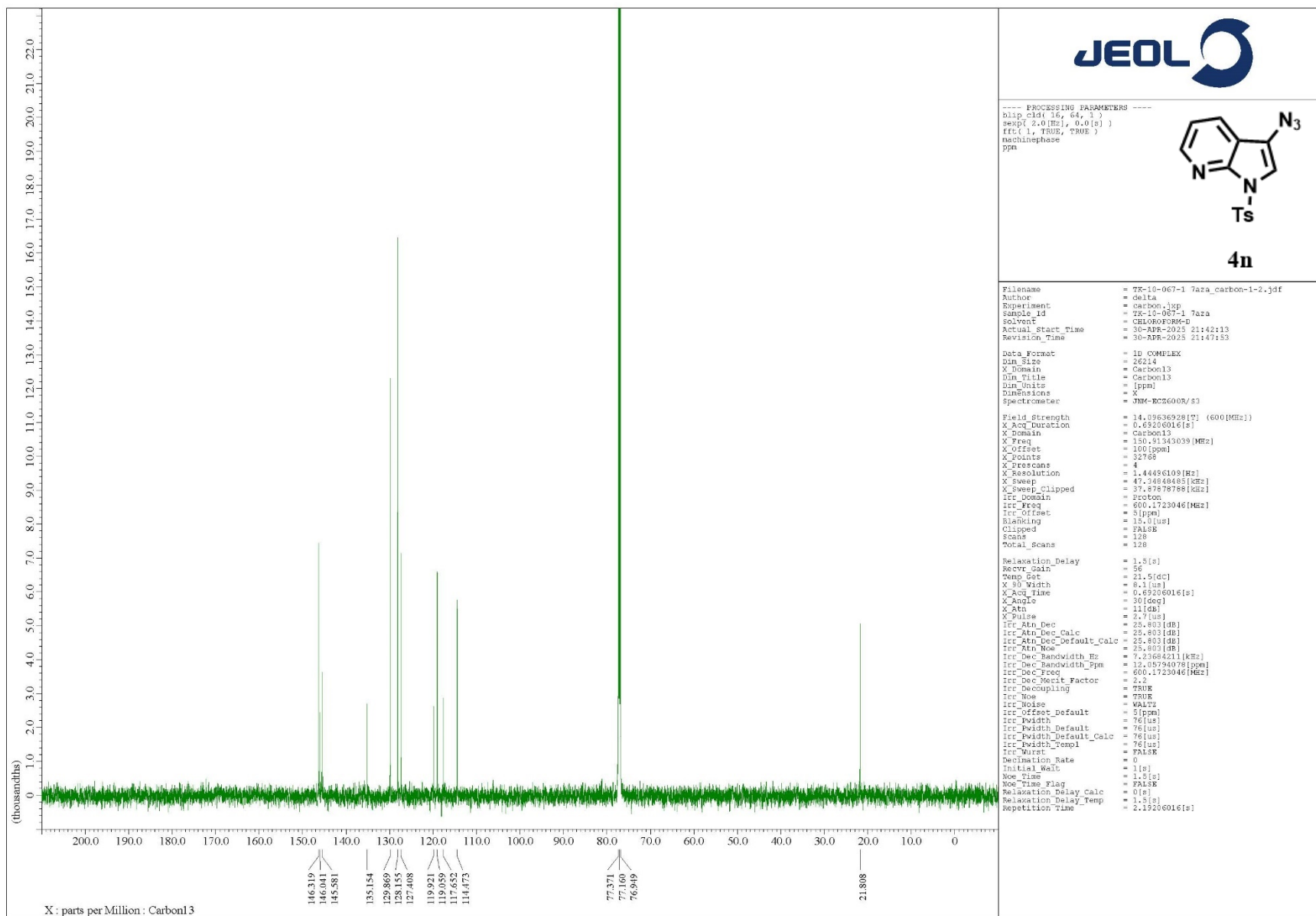


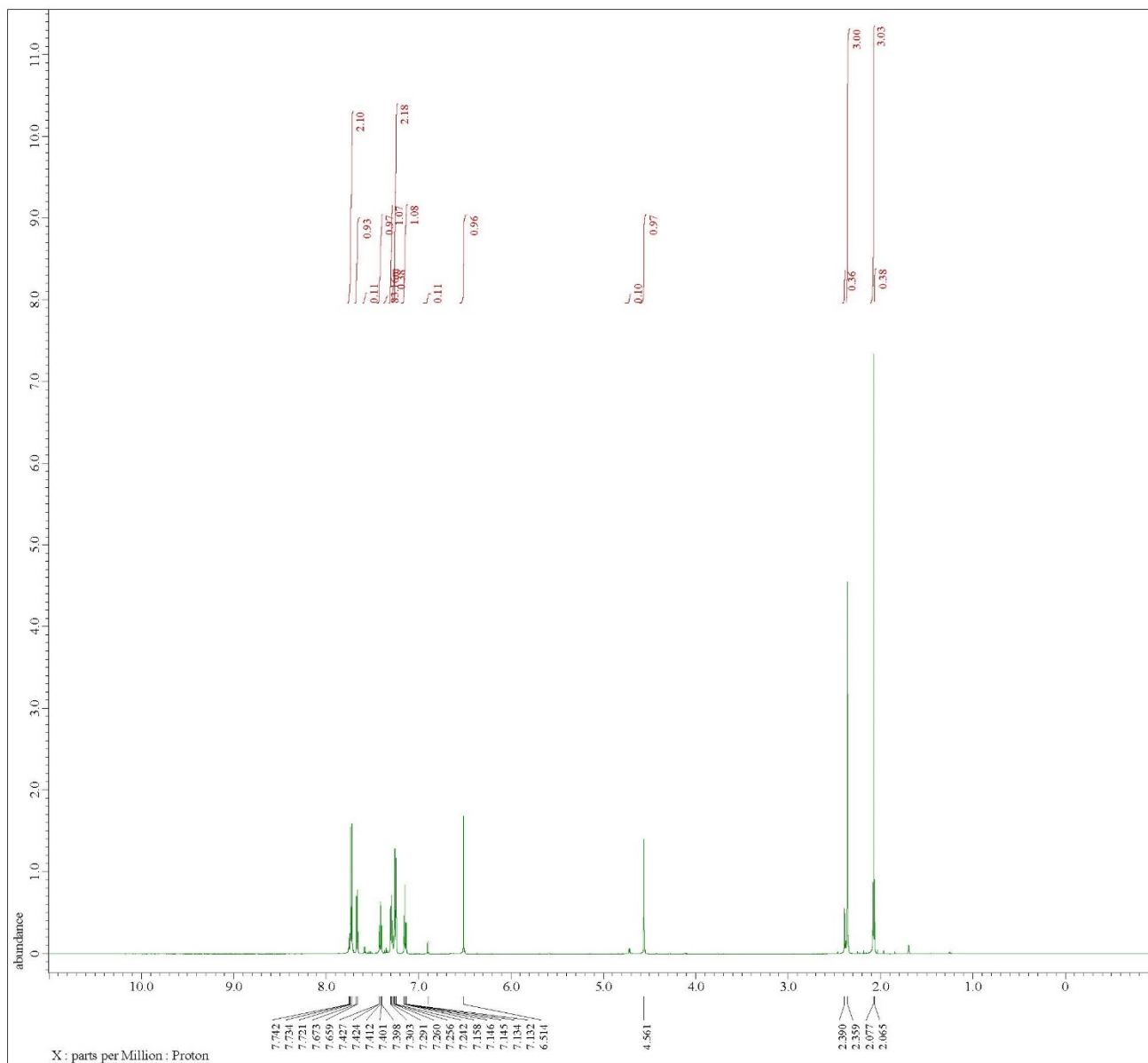
Filename = TK-10-067-1 7aza_proton-1-3.jdf
 Author = Delta
 Experiment = proton_3xp
 Sample_id = TK-10-067-1 7aza
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 30-APR-2025 21:41:17
 Revision_Time = 1-MAY-2025 22:32:13

Data_Format = 1D COMPLEX
 Din_Size = 26214
 X_Domain = Proton
 Din_Title = Proton
 Din_Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ600R/S3

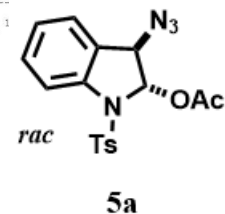
Field_Strength = 14.09636928[T] (600[MHz])
 X_Acq_Duration = 2.18103808[s]
 X_Domain = Proton
 X_Freq = 600.1723046[MHz]
 X_Offset = 8[ppm]
 X_Points = 32768
 X_Prescans = 1
 X_Resolution = 0.45849727[Hz]
 X_Sweep = 15.02403846[kHz]
 X_Sweep_Clipped = 12.01923077[kHz]
 ITC_Domain = Proton
 ITC_Freq = 600.1723046[MHz]
 ITC_Offset = 8[ppm]
 TCI_Domain = Proton
 TCI_Freq = 600.1723046[MHz]
 TCI_Offset = 8[ppm]
 Blanking = 5.0[us]
 Clipped = FALSE
 Scans = 4
 Total_Scans = 4

Relaxation_Delay = 2[s]
 Recvr_Gain = 56
 Temp_Set = 20.7[degC]
 X_90_Width = 10.5[us]
 X_Acq_Time = 2.18103808[s]
 X_Angle = 45[deg]
 X_Atn = 8.1[db]
 X_Pulse = 8.25[us]
 ITC_Mode = off
 TCI_Mode = off
 Danis_Loop = 200
 Danto_Preset = FALSE
 Decimation_Rate = 0
 Initial_Walt = 1[s]
 Phase = {0, 90, 270, 180, 180, 270, 90, 0}
 Preset_Time = 2[s]
 Preset_Time_Flag = FALSE
 Relaxation_Delay_Calc = 0[s]
 Relaxation_Delay_Temp = 2[s]
 Repetition_Time = 4.18103808[s]





--- PROCESSING PARAMETERS ---
 sepr(0.2[Hz], 0.0[F]
 trapezoid(0[%], 0[%], 80[%], 1
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinphase
 ppm

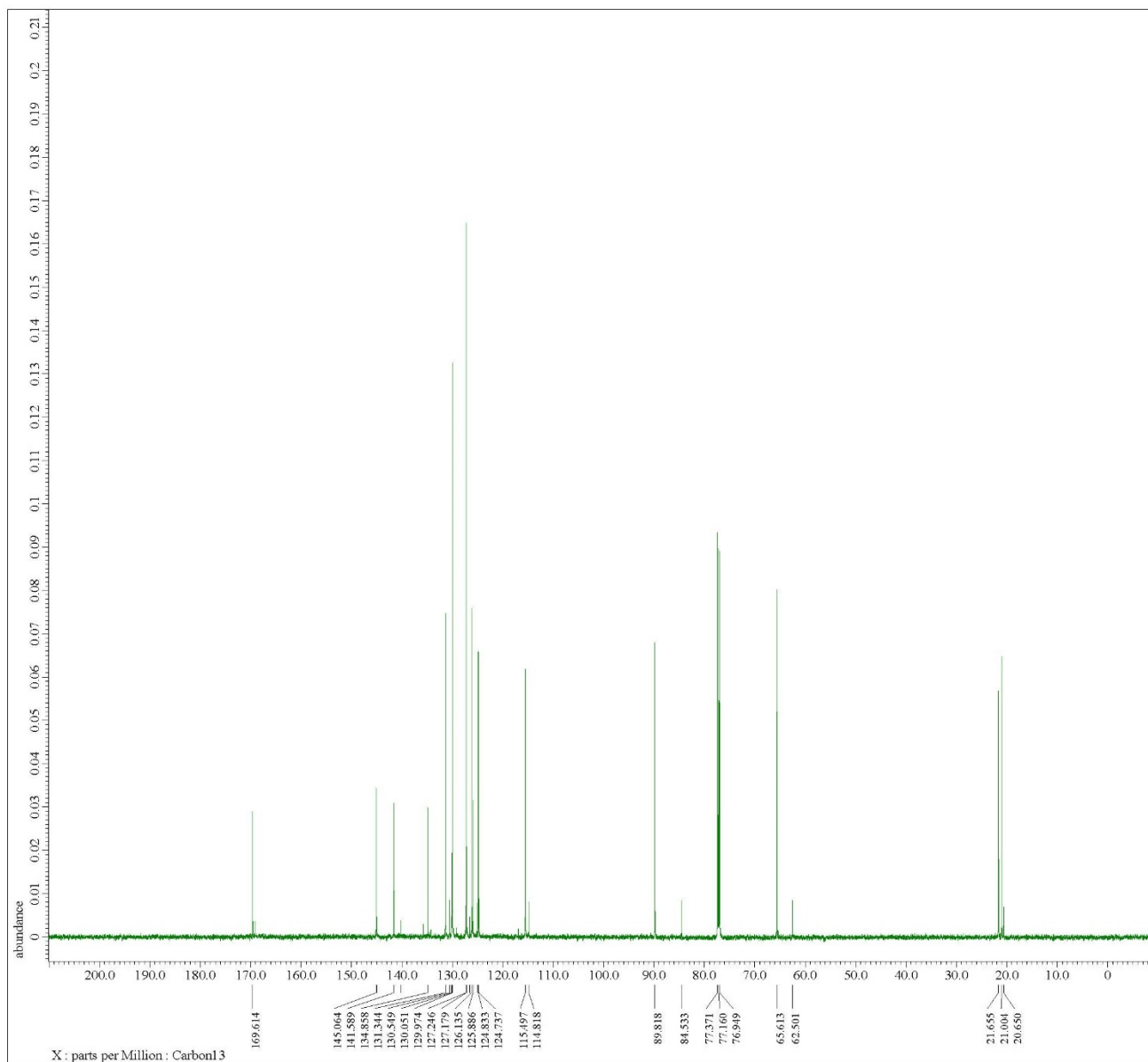


Filename = SR-2-025-1_proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample_id = SR-2-025-1
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 21-APR-2025 21:41:14
 Revision_Time = 27-MAY-2025 10:50:06

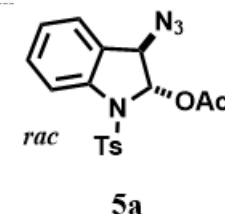
Data_Format = 1D COMPLEX
 Bin_Size = 36214
 X_Domain = Proton
 Bin_Title = Proton
 Bin_Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ600R/S3

Field_Strength = 14.09636928[T] (600[MHz])
 X_Acq_Duration = 2.18103808[s]
 X_Domain = Proton
 X_Freq = 600.1723046[MHz]
 X_Offset = 8[ppm]
 X_Points = 32768
 X_Prescans = 1
 X_Resolution = 0.45843727[Hz]
 Y_Sweep = 15.02403846[kHz]
 X_Sweep_Clipped = 12.01923077[kHz]
 F1_Domain = Proton
 F1_Freq = 600.1723046[MHz]
 F1_Offset = 8[ppm]
 F2_Domain = Proton
 F2_Freq = 600.1723046[MHz]
 F2_Offset = 8[ppm]
 Blanking = 5.0[us]
 Clipped = FALSE
 Scans = 4
 Total_Scans = 4

Relaxation_Delay = 2[s]
 Recv_Gain = 36
 Temp_Set = 21.3[degC]
 X_90_Width = 10.5[us]
 X_Acq_Time = 2.18103808[s]
 X_Angle = 45[deg]
 X_Atn = 8.1[db]
 X_Pulse = 8.25[us]
 T1R_Mode = Off
 T1R_Mode = Off
 Dntc_Loop = 200
 Dntc_Preset = FALSE
 Decimation_Rate = 0
 Initial_Walt = 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 ----
 disp.chdr 16, 64, 1
 seprf(2.0[MHz], 0.0[s])
 fft(1, TRUE, TRUE)
 machinephase
 ppm

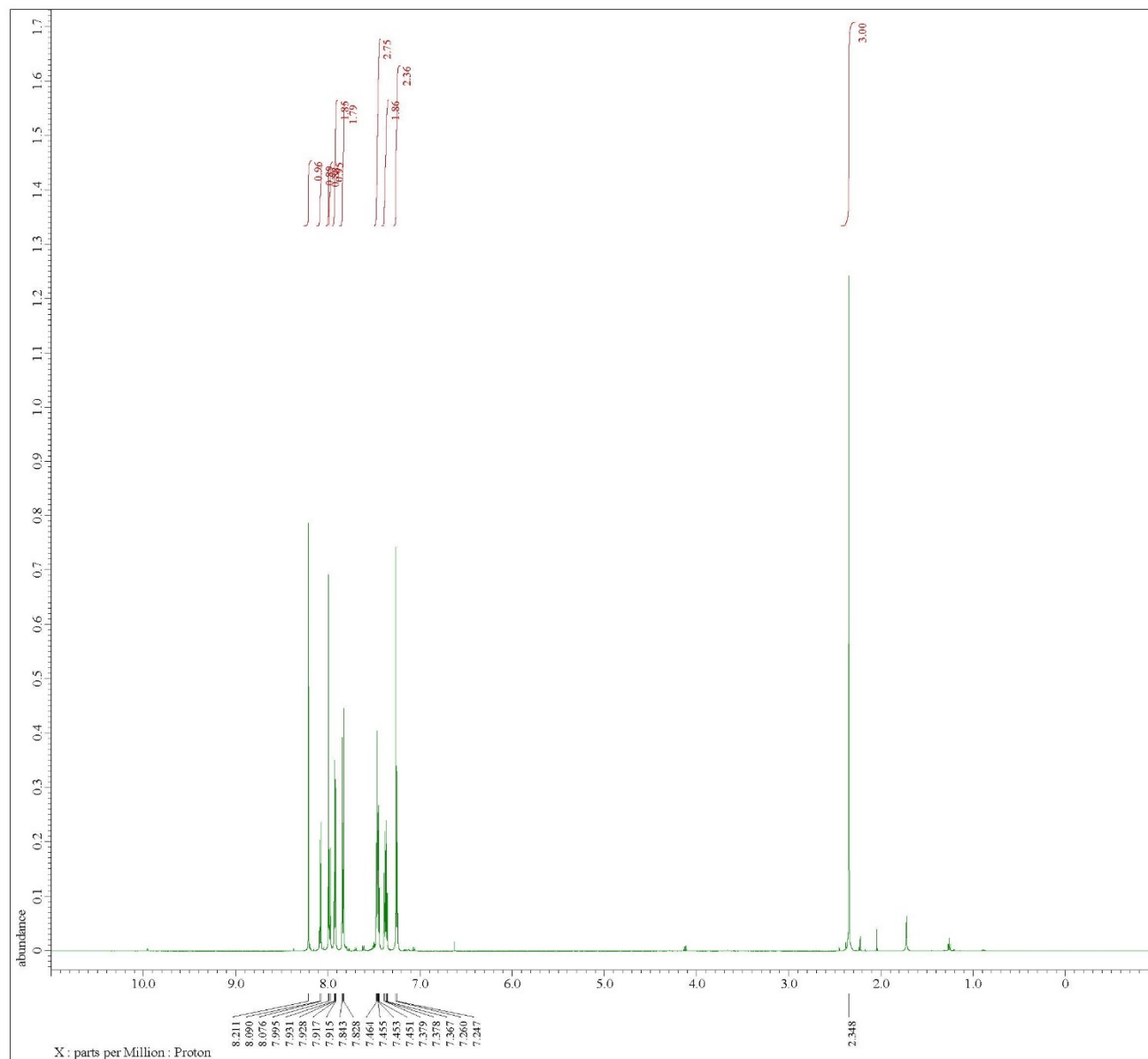


Filename = SA-2-025-1_carbon-1-2.ydf
 Author = delta
 Experiment = carbon13xp
 Sample_id = SA-2-025-1
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 21-APR-2025 21:43:32
 Revision_Time = 21-APR-2025 21:45:58

Data_Format = 1D COMPLEX
 Dm_Size = 26214
 X_Domain = Carbon13
 Dm_Title = Carbon13
 Dm_Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ600R/53

Field_Strength = 14.09636928[T] (600[MHz])
 X_Acq_Duration = 0.63206016[s]
 X_Domain = Carbon13
 X_Freq = 150.91343039[MHz]
 X_Offset = 100[ppm]
 X_Points = 32768
 X_Prescans = 4
 X_Resolution = 1.44456109[Hz]
 X_Sweep = 47.34848485[KHz]
 X_Sweep_Clipped = 37.87878788[KHz]
 Irc_Domain = Proton
 Irc_Freq = 600.1723046[MHz]
 Irc_Offset = 8[ppm]
 Binning = 15.0[us]
 Clipped = FALSE
 Scans = 40
 Total_Scans = 40

Relaxation_Delay = 1.5[s]
 Recvr_Gain = 56
 Temp_Get = 21[deg]
 X_90_Width = 8.1[us]
 X_Acq_Time = 0.63206016[s]
 X_Angle = 30[deg]
 X_Atn = 11[deg]
 X_Pulse = 2.7[us]
 Irc_Atn_Dec = 25.803[deg]
 Irc_Atn_Dec_Calc = 25.803[deg]
 Irc_Atn_Dec_Default_Calc = 25.803[deg]
 Irc_Atn_Noise = 25.803[deg]
 Irc_Dec_Bandwidth_Hz = 7.23684211[KHz]
 Irc_Dec_Bandwidth_Ppm = 12.05794078[ppm]
 Irc_Dec_Freq = 600.1723046[MHz]
 Irc_Dec_Merit_Factor = 2.2
 Irc_Decoupling = TRUE
 Irc_Noise = TRUE
 Irc_Noise_Default = WALTZ
 Irc_Offset_Default = 5[ppm]
 Irc_Pwidth = 76[us]
 Irc_Pwidth_Default = 76[us]
 Irc_Pwidth_Default_Calc = 76[us]
 Irc_Pwidth_Templ = 76[us]
 Irc_Wurst = FALSE
 Declination_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 = 2.12206016[s]



```

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

```

```

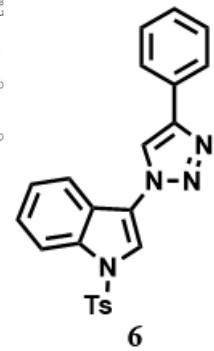
Filename      = SA-2-002-main_proton-1-3.jdf
Author        = delta
Experiment    = proton.jxp
Sample_id     = SA-2-002-main
Solvent       = CHLOROFORM-D
Actual_Start_Time = 30-APR-2025 22:12:04
Revision_Time  = 1-MAY-2025 22:37:43

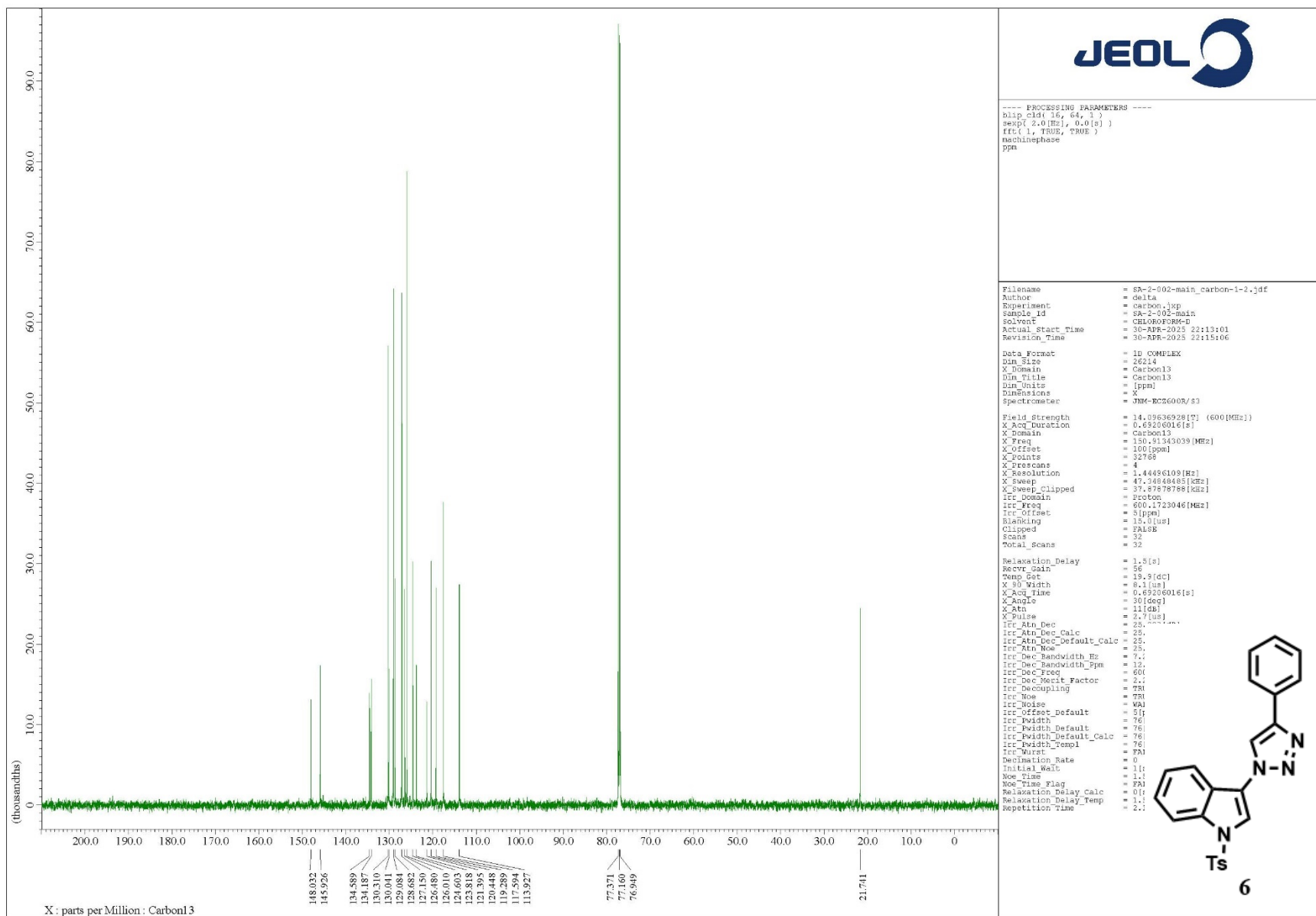
Data_Format   = 1D COMPLEX
Dir_Size      = 26214
X_Domain      = Proton
Dir_Title     = Proton
Dir_Units     = [ppm]
Dimensions    = 2
Spectrometer  = JNM-ECZ600R/S3

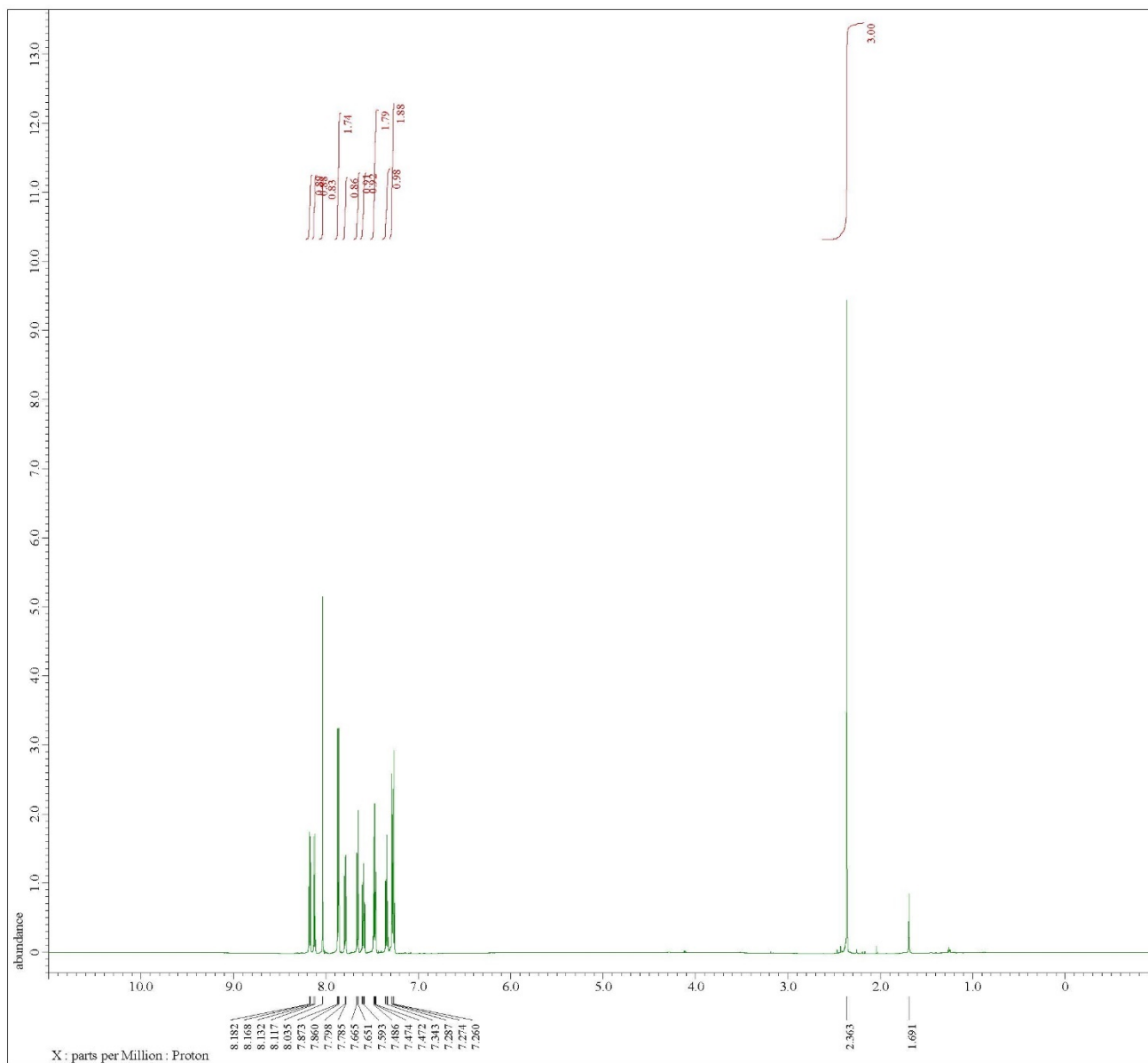
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain       = Proton
X_Freq         = 600.1723046[MHz]
X_Offset       = 8[ppm]
X_Points       = 32768
X_Prescans     = 1
X_Resolution   = 0.45849727[Hz]
X_Sweep        = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
Irr_Domain     = Proton
Irr_Freq       = 600.1723046[MHz]
Irr_Offset     = 8[ppm]
Tc1_Domain     = Proton
Tc1_Freq       = 600.1723046[MHz]
Tc1_Offset     = 8[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_scans    = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 36
Temp_Set        = 19.9[degC]
X_90_Width      = 10.5[us]
X_Acq_Time      = 2.18103808[s]
X_Angle         = 45[deg]
X_Atn           = 8.1[db]
X_Pulse         = 8.25[us]
Irr_Mode        = off
Tc1_Mode        = off
Dante_Loop      = 200
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase           = {0, 90}
Preset_Time     = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.1810

```







```

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

```

```

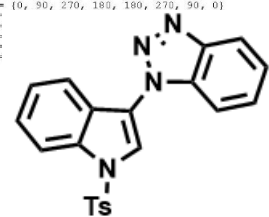
Filename      = SR-2-006-main_proton-1-3.jdf
Author        = delta
Experiment    = proton.jxp
Sample_id     = SR-2-006-main
Solvent       = CHLOROFORM-D
Actual_Start_Time = 30-APR-2025 22:18:57
Revision_Time  = 1-MAY-2025 22:41:15

Data_Format   = 1D COMPLEX
Bin_Size      = 26214
X_Domain      = Proton
Bin_Title     = Proton
Bin_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ600R/S3

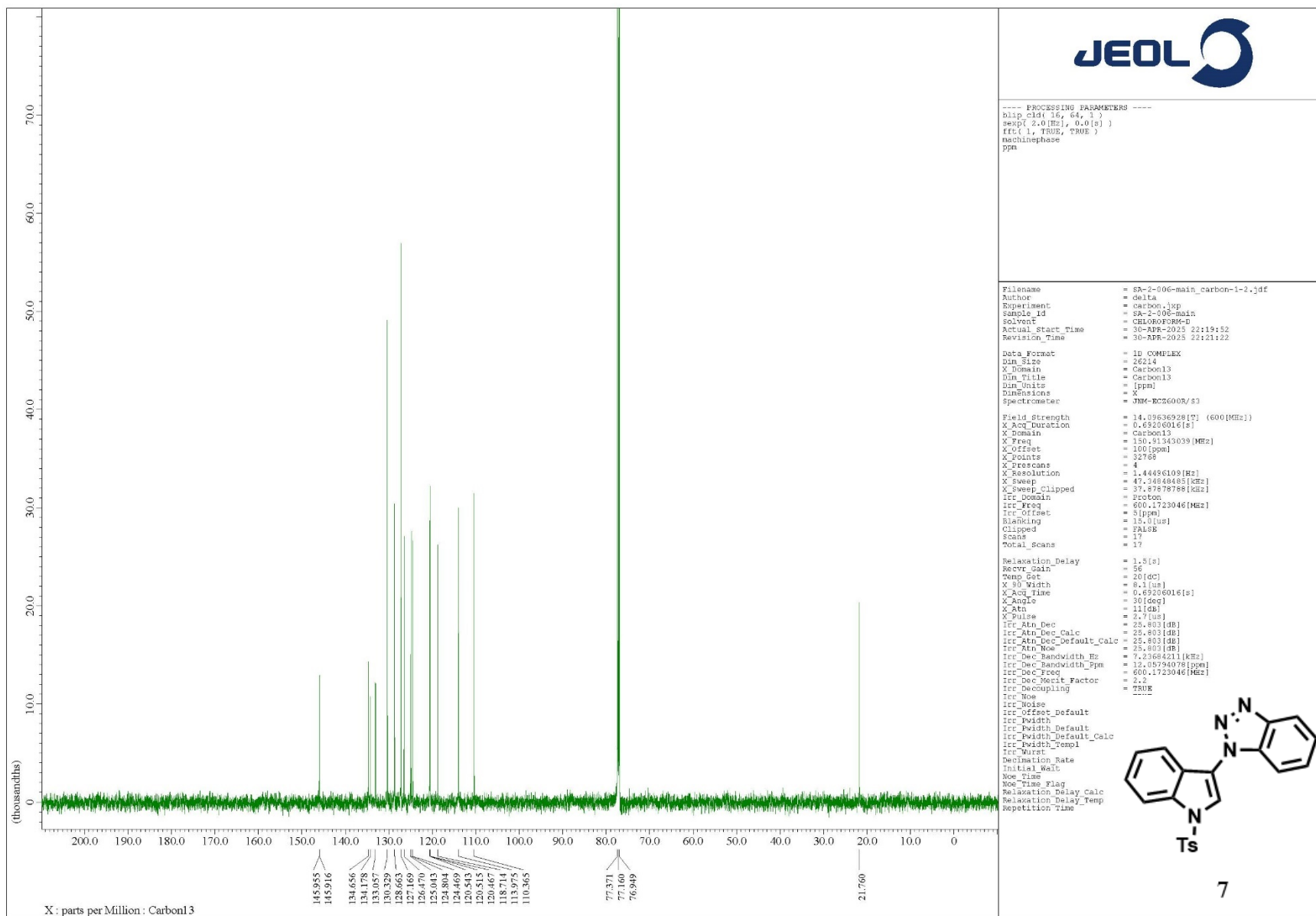
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain       = Proton
X_Freq         = 600.1723046[MHz]
X_Offset       = 5[ppm]
X_Points       = 32768
X_Prescans     = 1
X_Resolution   = 0.45843727[Hz]
Y_Sweep        = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
F1_Domain      = Proton
F1_Freq        = 600.1723046[MHz]
F1_Offset      = 5[ppm]
T1_Domain      = Proton
T1_Freq        = 600.1723046[MHz]
T1_Offset      = 5[ppm]
Blanking       = 5.0[us]
Clipped        = TRUE
Scans          = 4
Total_Scans    = 4

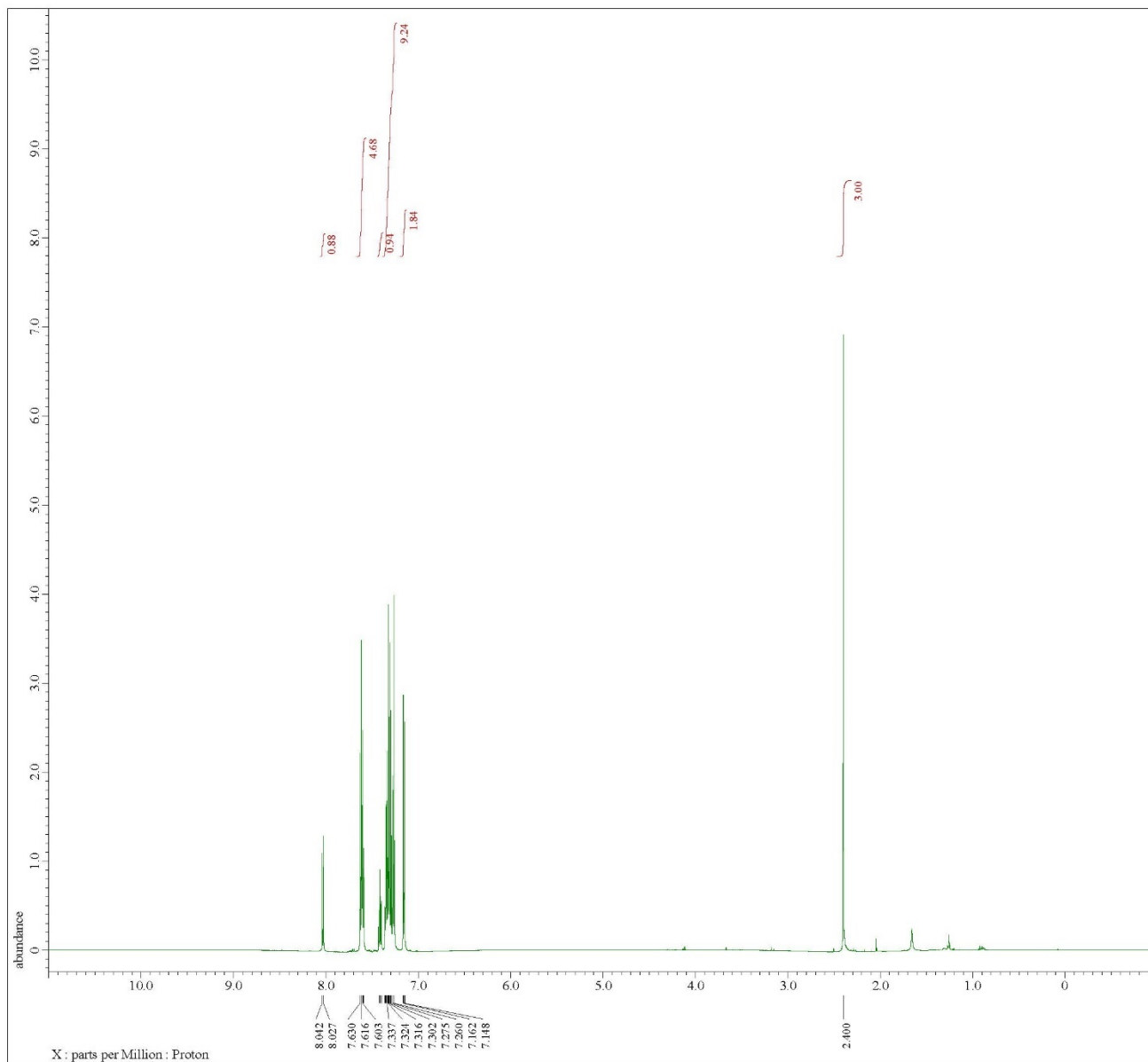
Relaxation_Delay = 2[s]
Recvr_Gain       = 26
Temp_Set        = 19.9[degC]
X_90_Width      = 10.5[us]
X_Acq_Time      = 2.18103808[s]
X_Angle         = 45[deg]
X_Atn          = 8.1[db]
X_Pulse         = 8.25[us]
F1_Mode         = Off
T1_Mode         = Off
Dante_Loop      = 200
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Walt    = 1[s]
Phase           = {0, 90, 270, 180, 270, 90, 0}
Preset_Time     =
Preset_Time_Flag =
Relaxation_Delay_Calc =
Relaxation_Delay_Temp =
Repetition_Time =

```



7





```

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

```

```

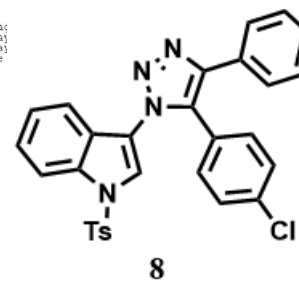
Filename      = SA-2-016-main_proton-1-3.jdf
Author        = delta
Experiment    = proton.jpg
Sample_ID     = SA-2-016-main
Solvent       = CHLOROFORM-D
Actual_Start_Time = 30-APR-2025 22:24:06
Revision_Time = 1-MAY-2025 22:43:39

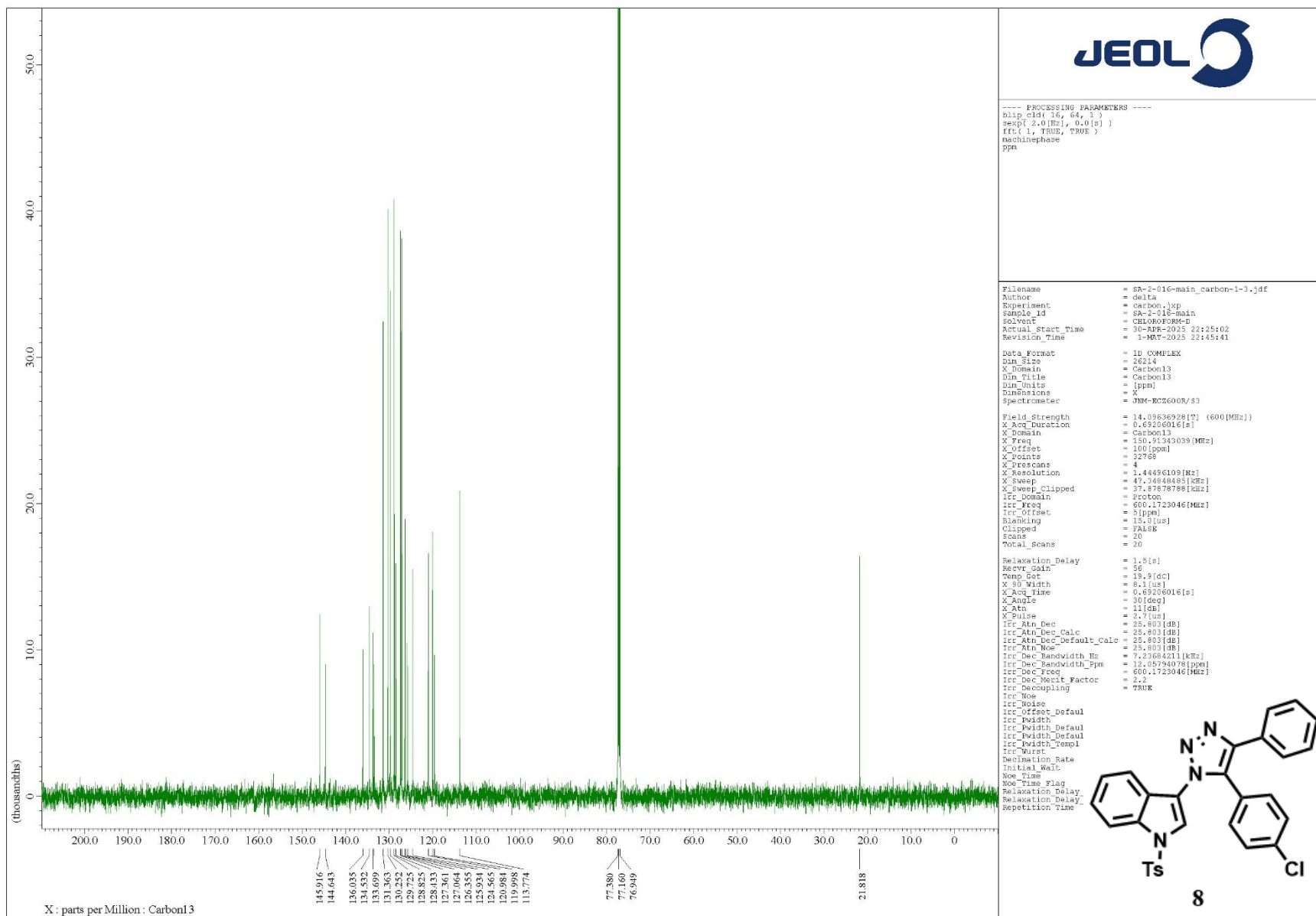
Data_Format   = 1D REAL
DIN_Size      = 26214
X_Domain      = Proton
DIN_Title     = Proton
DIN_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ600R/S3

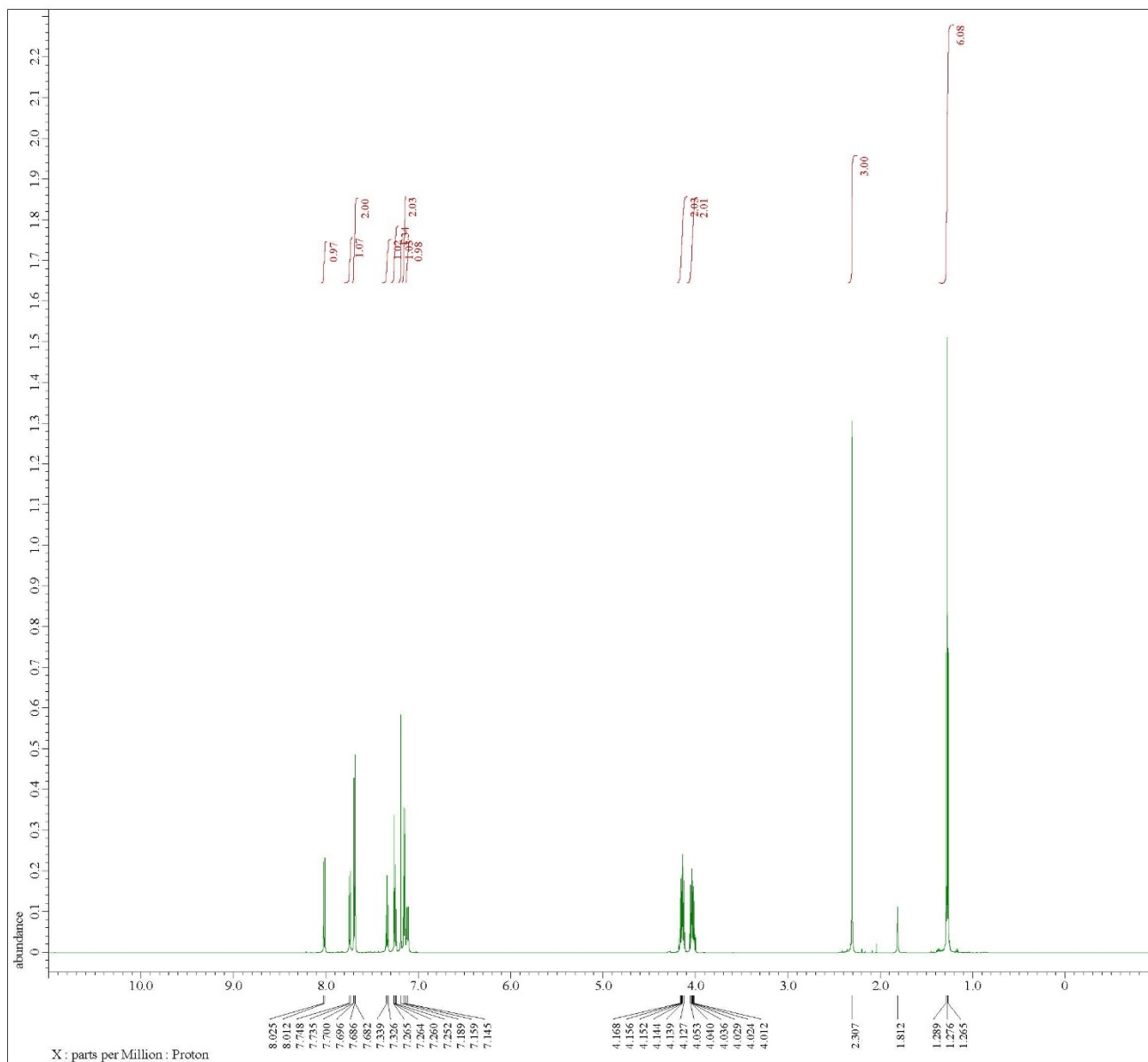
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain       = Proton
X_Freq         = 600.1723046[MHz]
X_Offset       = 5[ppm]
X_Points       = 32768
X_Prescans     = 1
X_Resolution   = 0.45849727[Hz]
X_Sweep        = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
IF1_Domain     = Proton
IF1_Freq       = 600.1723046[MHz]
IF1_Offset     = 5[ppm]
TC1_Domain     = Proton
TC1_Freq       = 600.1723046[MHz]
TC1_Offset     = 5[ppm]
Blanking       = 5.0[us]
Clipped        = TRUE
Scans          = 4
Total_Scans    = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 56
Temp_Set         = 19.9[degC]
X_90_Width       = 10.5[us]
X_Acq_Time       = 2.18103808[s]
X_Angle          = 45[deg]
X_Atn            = 8.1[deg]
X_Pulse          = 5.25[us]
IF1_Mode         = Off
TC1_Mode         = Off
DANTE_Loop       = 200
DANTE_Preset     = FALSE
Decimation_Rate  = 0
Initial_Wait     = 1[s]
Phase            =
Preset_Time      =
Preset_Time_Flag =
Relaxation_Delay =
Relaxation_Delay =
Repetition_Time  =

```







```

---- PROCESSING PARAMETERS ----
sext( 0.2[Hz], 0.0[F] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinphase
ppm

```

```

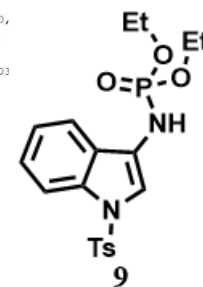
Filename      = SR-2-014-3-fca14_proton-1-3.jdf
Author        = delta
Experiment    = proton.jpg
Sample_id     = SR-2-014-3-fca14
Solvent       = CHLOROFORM-D
Actual_Start_Time = 1-MAY-2025 21:47:36
Revision_Time = 1-MAY-2025 22:49:36

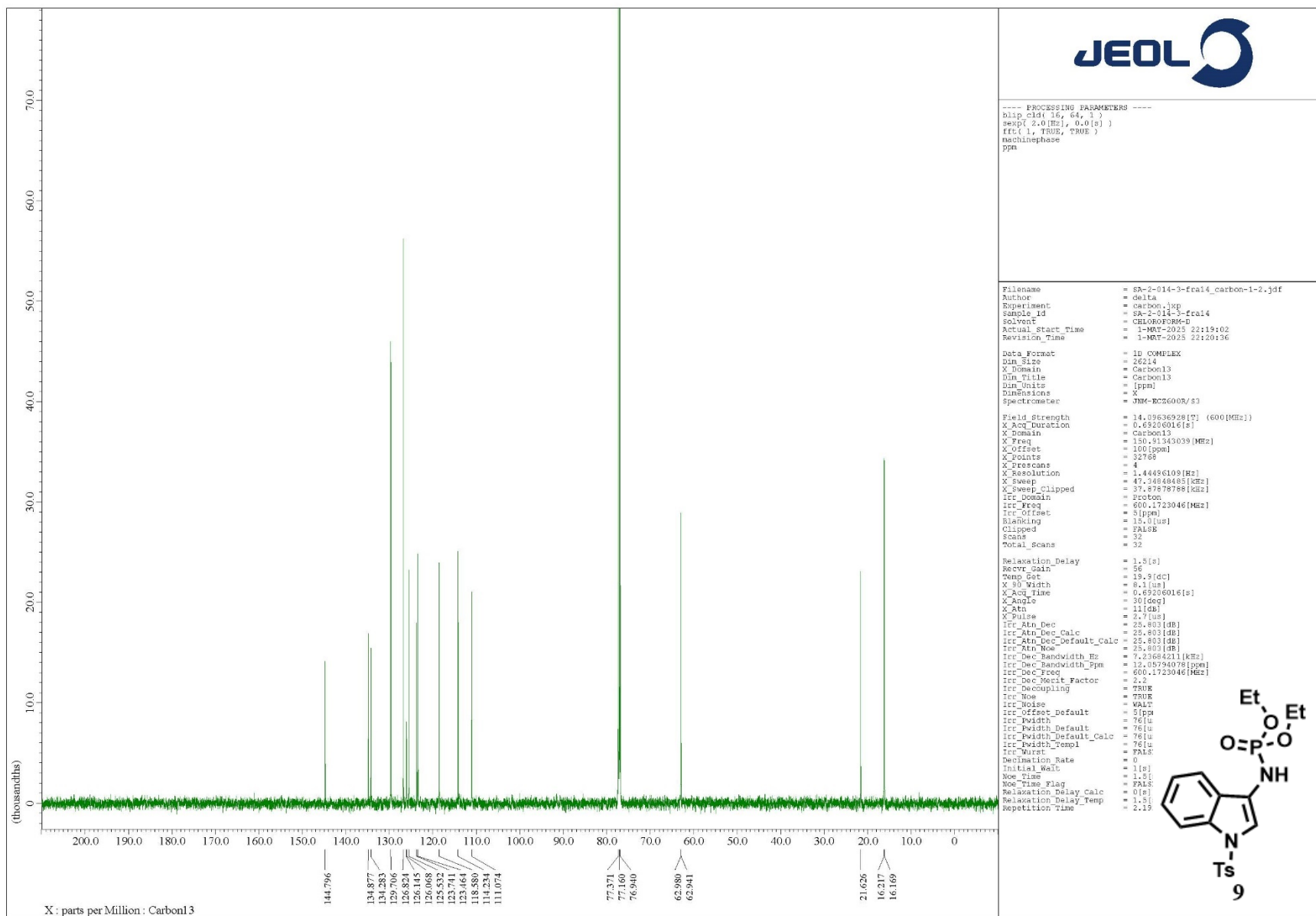
Data Format    = 1D COMPLEX
Dim Size      = 36214
X_Domain      = Proton
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = 1
Spectrometer  = JNM-ECZ600R/S3

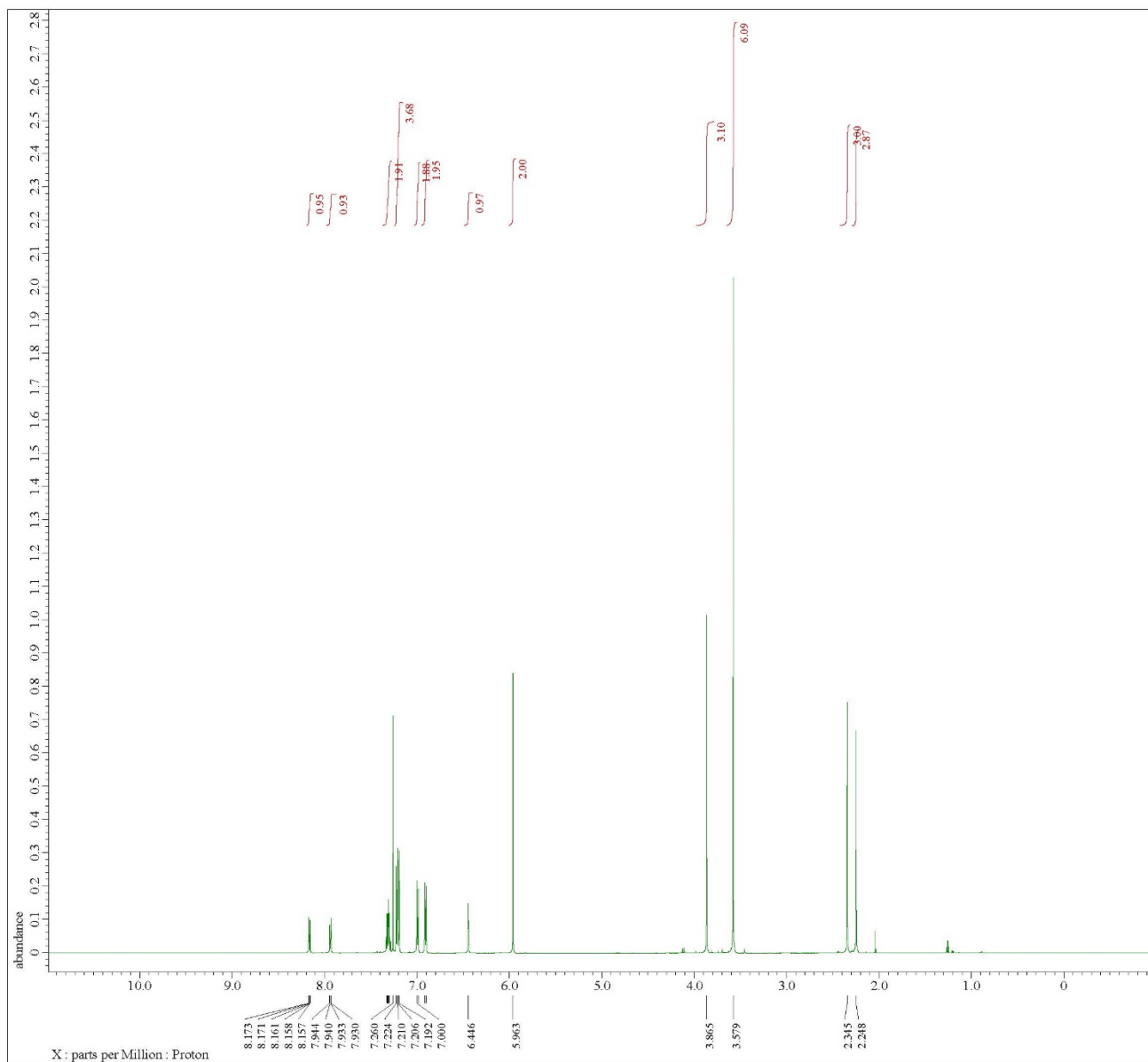
Field Strength = 14.09636928[T] (600[MHz])
X_Acq Duration = 2.18103808[s]
X_Domain       = Proton
X_Freq         = 600.1723046[MHz]
X_Offset       = 5[ppm]
X_Points       = 32768
X_Prescans     = 1
X_Resolution   = 0.43849727[Hz]
X_Sweep        = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
F1_Domain      = Proton
F1_Freq        = 600.1723046[MHz]
F1_Offset      = 5[ppm]
F2_Domain      = Proton
F2_Freq        = 600.1723046[MHz]
F2_Offset      = 5[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_Scans    = 4

Relaxation_Delay = 2[s]
Recvr Gain       = 36
Temp_Set         = 20[degC]
X_90_Width       = 10.5[us]
X_Acq Time       = 2.18103808[s]
X_Angle          = 45[deg]
X_Attn           = 8.1[dB]
X_Pulse          = 6.25[us]
TEC Mode        = Off
TEC Mode        = Off
Dante Loop      = On
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Wait     = 1[s]
Phase           = {0, 90,
Preset_Time     = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18103

```







```

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

```

```

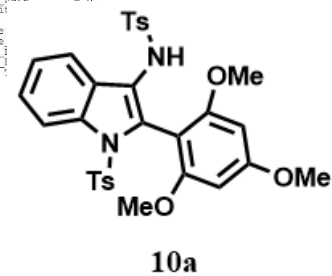
Filename      = SR-2-053-fra21-25_proton-1-3.jdf
Author        = delta
Experiment    = proton.jpg
Sample_id     = SR-2-053-fra21-25
Solvent       = CHLOROFORM-D
Actual_Start_Time = 12-MAY-2025 22:24:32
Revision_Time = 27-MAY-2025 09:44:59

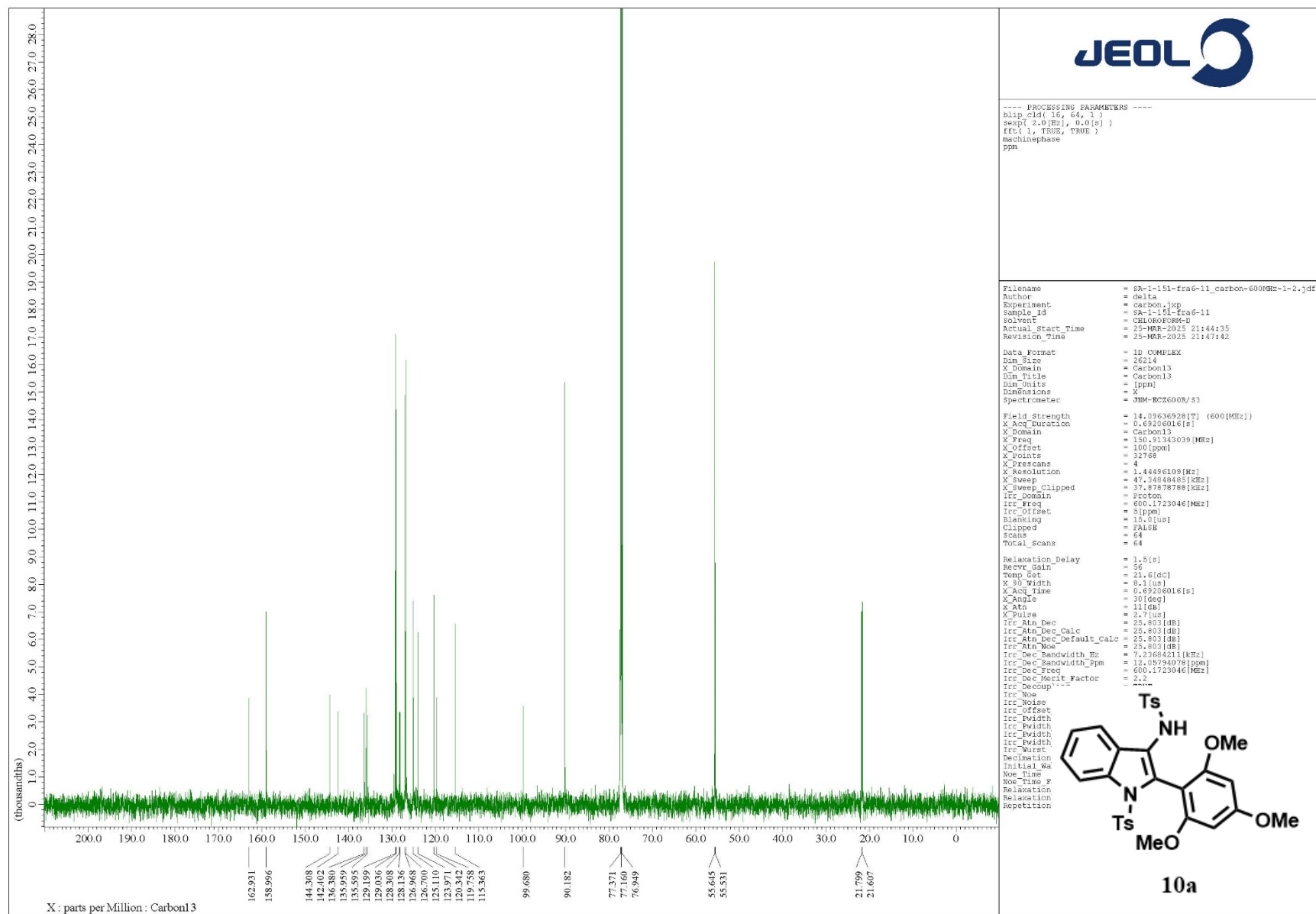
Data_Format   = 1D_COMPLEX
Bin_Size      = 26214
X_Domain      = Proton
Bin_Title     = Proton
Bin_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ600R/S3

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]
f1c_Domain    = Proton
f1c_Freq      = 600.1723046[MHz]
f1c_Offset    = 5[ppm]
f2c_Domain    = Proton
f2c_Freq      = 600.1723046[MHz]
f2c_Offset    = 5[ppm]
Blanking      = 5.0[us]
Clipped       = FALSE
Scans         = 4
Total_Scans   = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 26
Temp_Set         = 20.1[degC]
X_90_Width       = 10.5[us]
X_Acq_Time       = 2.18103808[s]
X_Angle          = 45[deg]
X_Attn           = 8.1[dB]
X_Pulse          = 6.25[us]
TEC_Mode         = Off
TEC_Temp         = Off
Dante_Loop       = Off
Dante_Preset     = FALSE
Decimation_Factor = n
Initial_Wait     = Phase
Preset_Time      = Preset_Time
Relaxation_1     = Relaxation_1
Relaxation_2     = Relaxation_2
Repetition_1     = Repetition_1

```

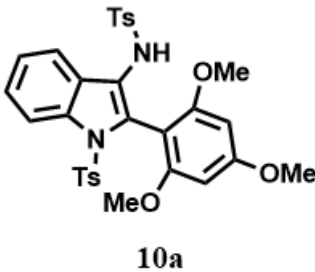


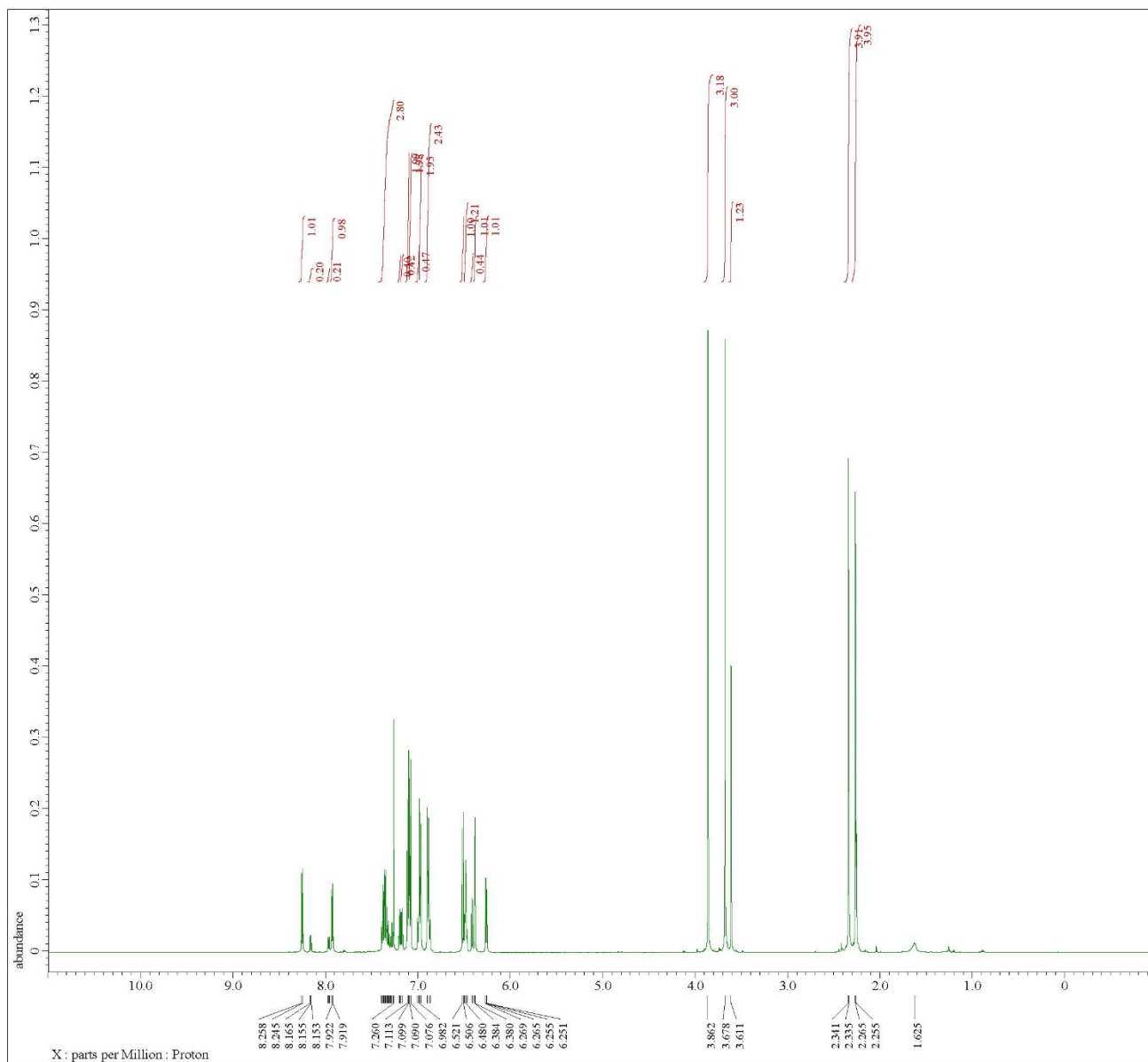


```

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

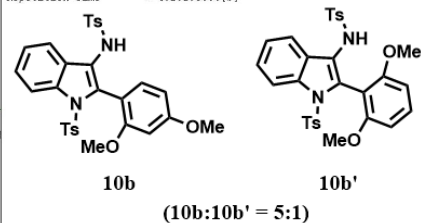
```

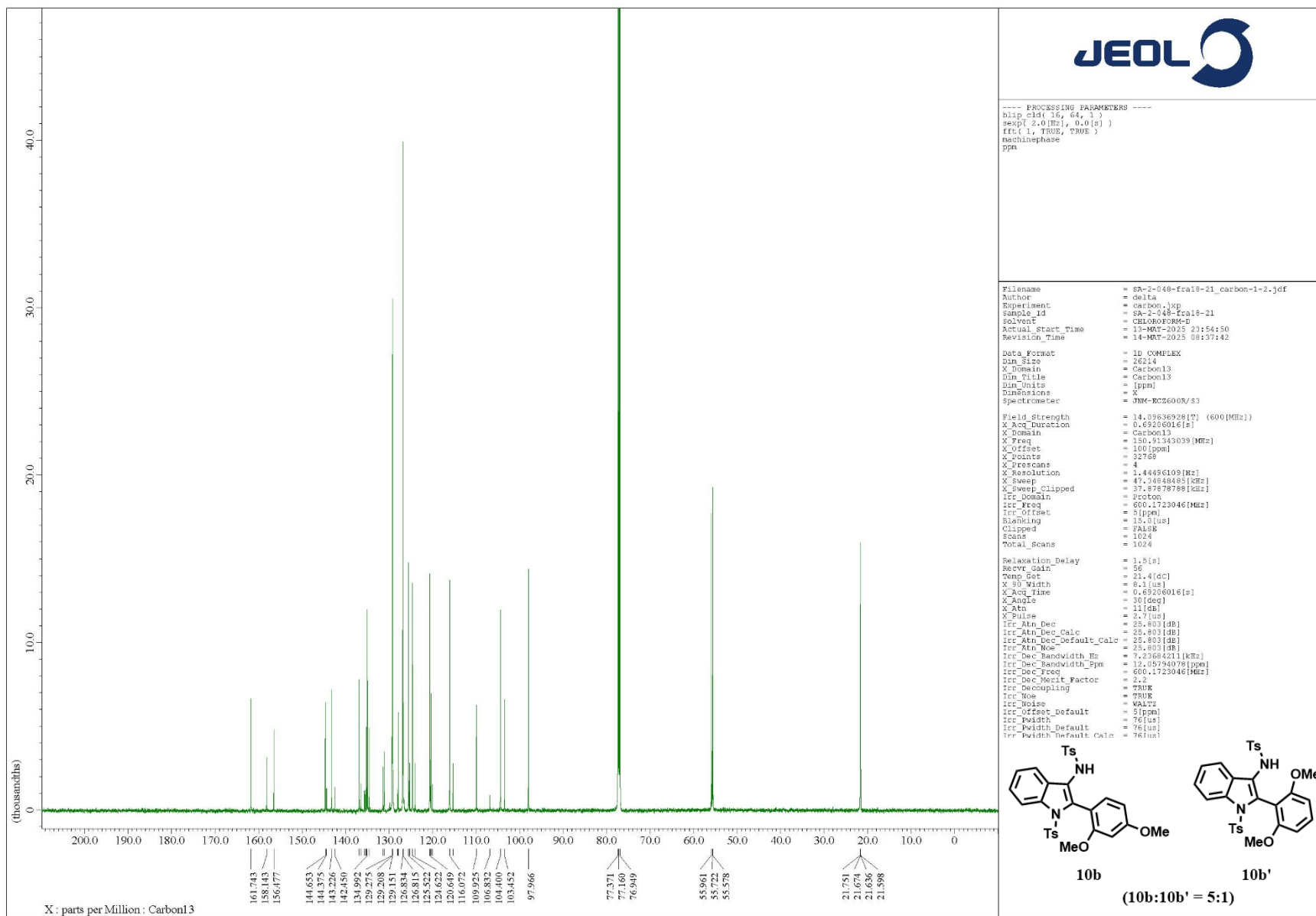
[illegible]

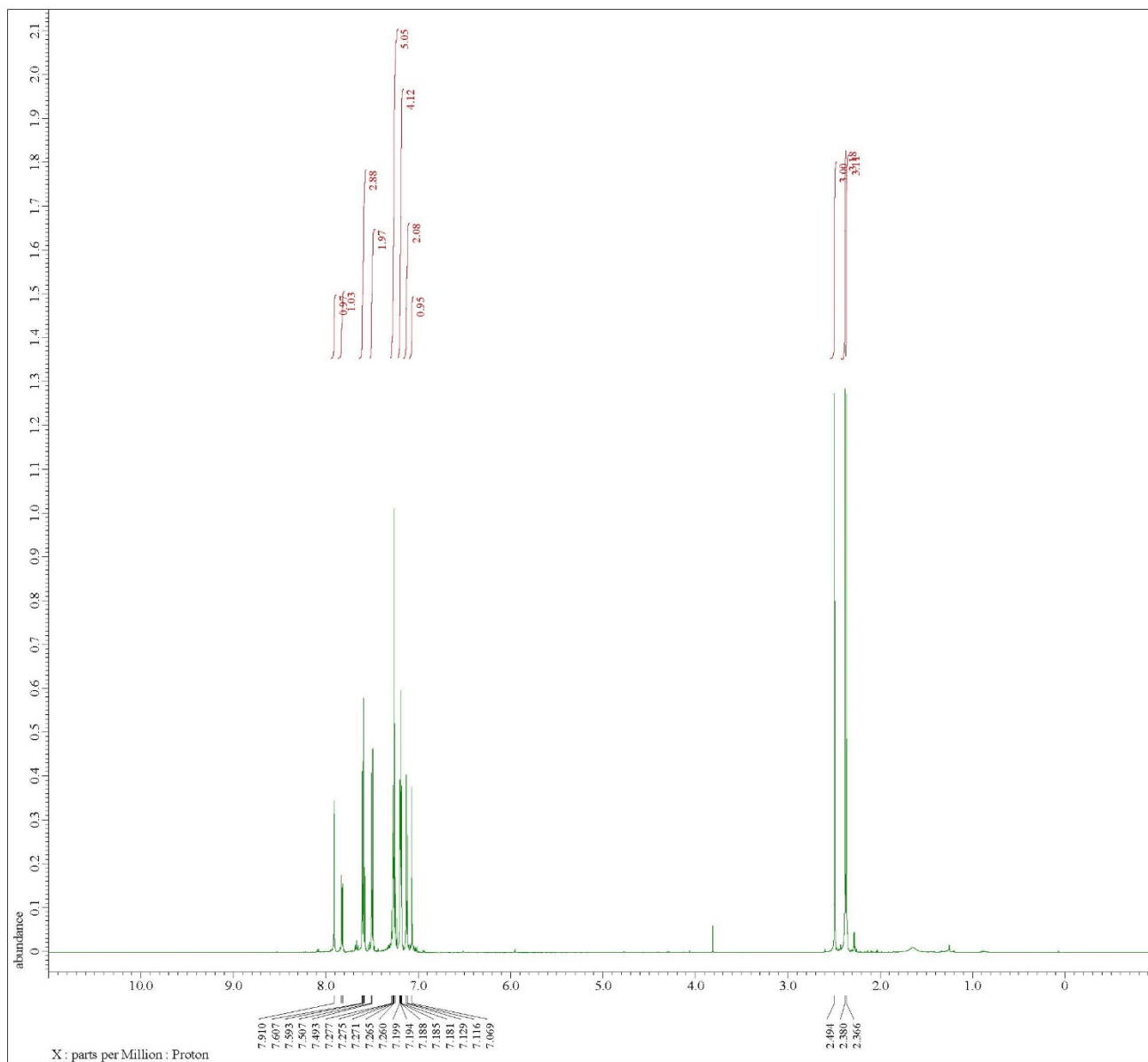


---- PROCESSING PARAMETERS ----
 smpc(0.2[Hz], 0.0[F])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 f2c(1, TRUE, TRUE)
 machinephase
 ppm
 reference(7.24905[ppm], 7.26[ppm])
 thresh(0.70202[%], 1,)
 以下由来: SA-2-048-fra18-21 proton-2-1.jdf

Filename = SA-2-048-fra18-21_proton-2-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample_id = SA-2-048-fra18-21
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 13-MAY-2025 22:55:17
 Revision_Time = 27-MAY-2025 10:29:14
 Data_Format = 1D COMPLEX
 Bin_Size = 36214
 X_Domain = Proton
 Din_Title = Proton
 Din_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 = 0.43849727[Hz]
 X_Sweep = 15.02403846[kHz]
 X_Sweep_Clipped = 12.01923077[kHz]
 Ict_Domain = Proton
 Ict_Freq = 600.1723046[MHz]
 Ict_Offset = 5[ppm]
 Tel_Domain = Proton
 Tel_Freq = 600.1723046[MHz]
 Tel_Offset = 5[ppm]
 Blanking = 5.0[us]
 Clipped = FALSE
 Scans = 4
 Total_Scans = 4
 Relaxation_Delay = 2[s]
 Recvr_Gain = 36
 Temp_Set = 19.6[deg]
 X_90_Width = 10.5[us]
 X_Acq_Time = 2.18103808[s]
 X_Angle = 45[deg]
 X_Atn = 8.1[db]
 X_Pulse = 6.25[us]
 T1c_Mode = Off
 T1c_Leop = 200
 Dantc_Preset = 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 ----
sexpr( 0.2[Hz], 0.0[F] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

```

```

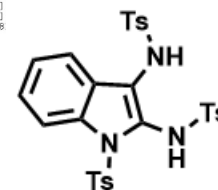
Filename      = SR-2-042-PTLC_proton-1-3.pdf
Author        = delta
Experiment    = proton_1xp
Sample_id     = SR-2-042-PTLC
Solvent       = CHLOROFORM-D
Actual_Start_Time = 12-MAY-2025 22:15:58
Revision_Time  = 27-MAY-2025 10:34:37

Data Format    = 1D COMPLEX
Dim Size      = 26214
X_Domain      = Proton
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = 1
Spectrometer  = JNM-ECZ600R/S3

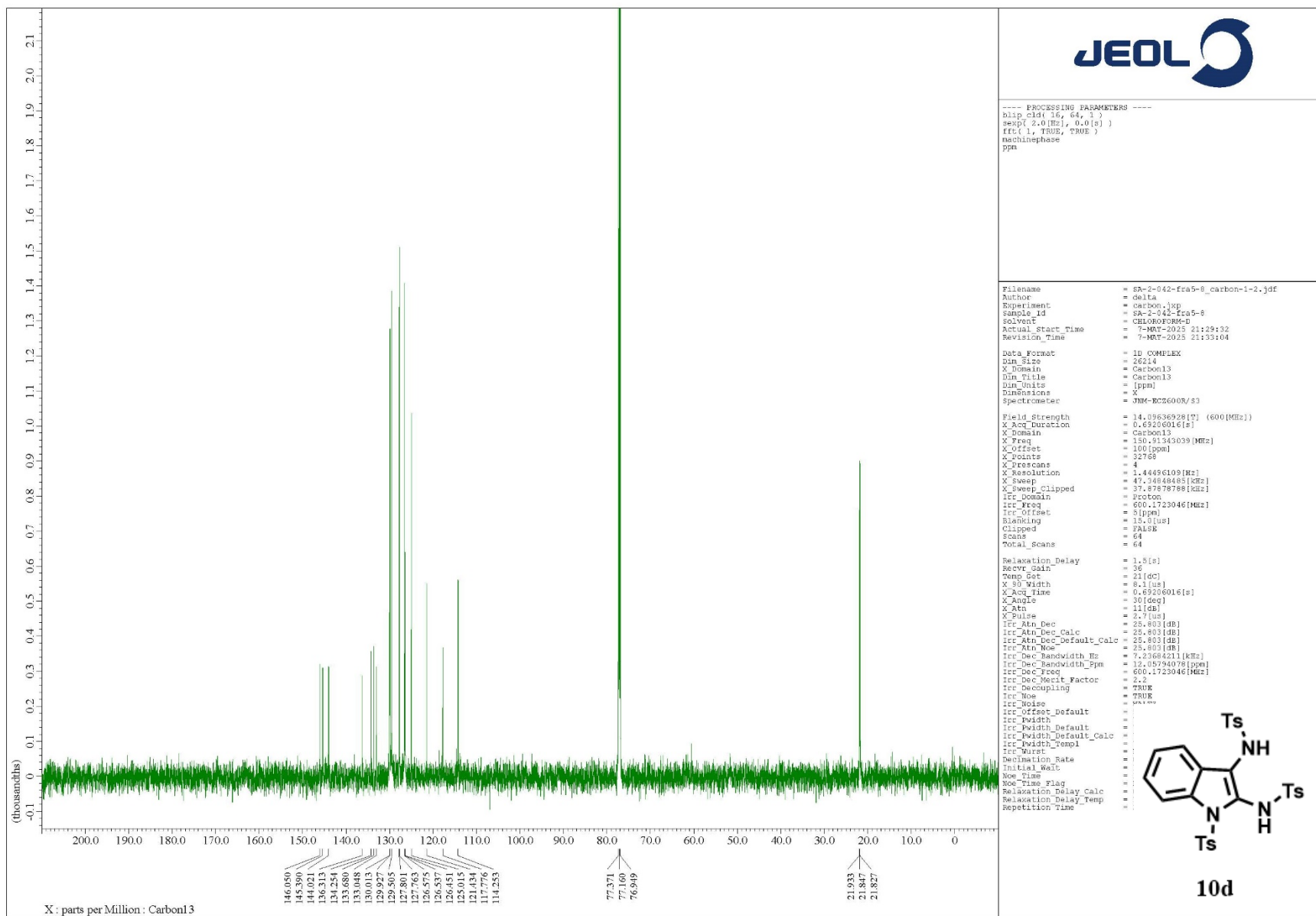
Field Strength = 14.09636928[T] (600[MHz])
X_Acq Duration = 2.18103808[s]
X_Domain      = Proton
X_Freq        = 600.1723046[MHz]
X_Offset      = 5[ppm]
X_Points      = 32768
X_Prescans    = 1
X_Resolution  = 0.43849727[Hz]
X_Sweep       = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
F1_Domain     = Proton
F1_Freq       = 600.1723046[MHz]
F1_Offset     = 5[ppm]
F2_Domain     = Proton
F2_Freq       = 600.1723046[MHz]
F2_Offset     = 5[ppm]
Blanking      = 5.0[us]
Clipped       = FALSE
Scans         = 4
Total_Scans   = 4

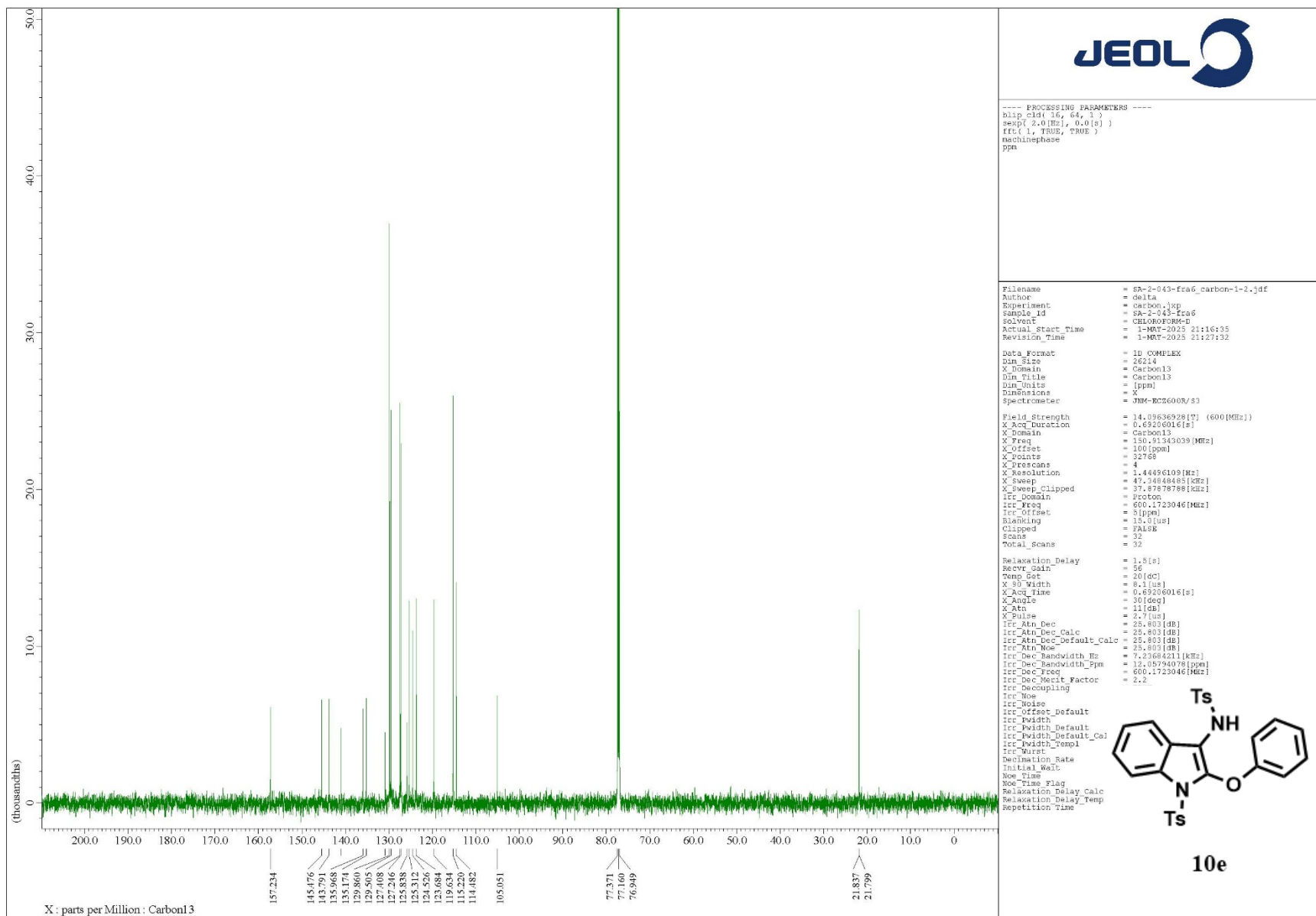
Relaxation_Delay = 2[s]
Recvr Gain      = 26
Temp_Set       = 20.5[degC]
X_90_Width     = 10.5[us]
X_Acq Time     = 2.18103808[s]
X_Angle        = 45[deg]
X_Attn         = 8.1[dB]
X_Pulse        = 5.25[us]
TEC Mode       = Off
TEC Mode       = Off
Dante_Loop     = 200
Dante_Preset   = FALSE
Decimation_Rate = 0
Initial_Wait   = 1[s]
Phase          = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time    = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.18

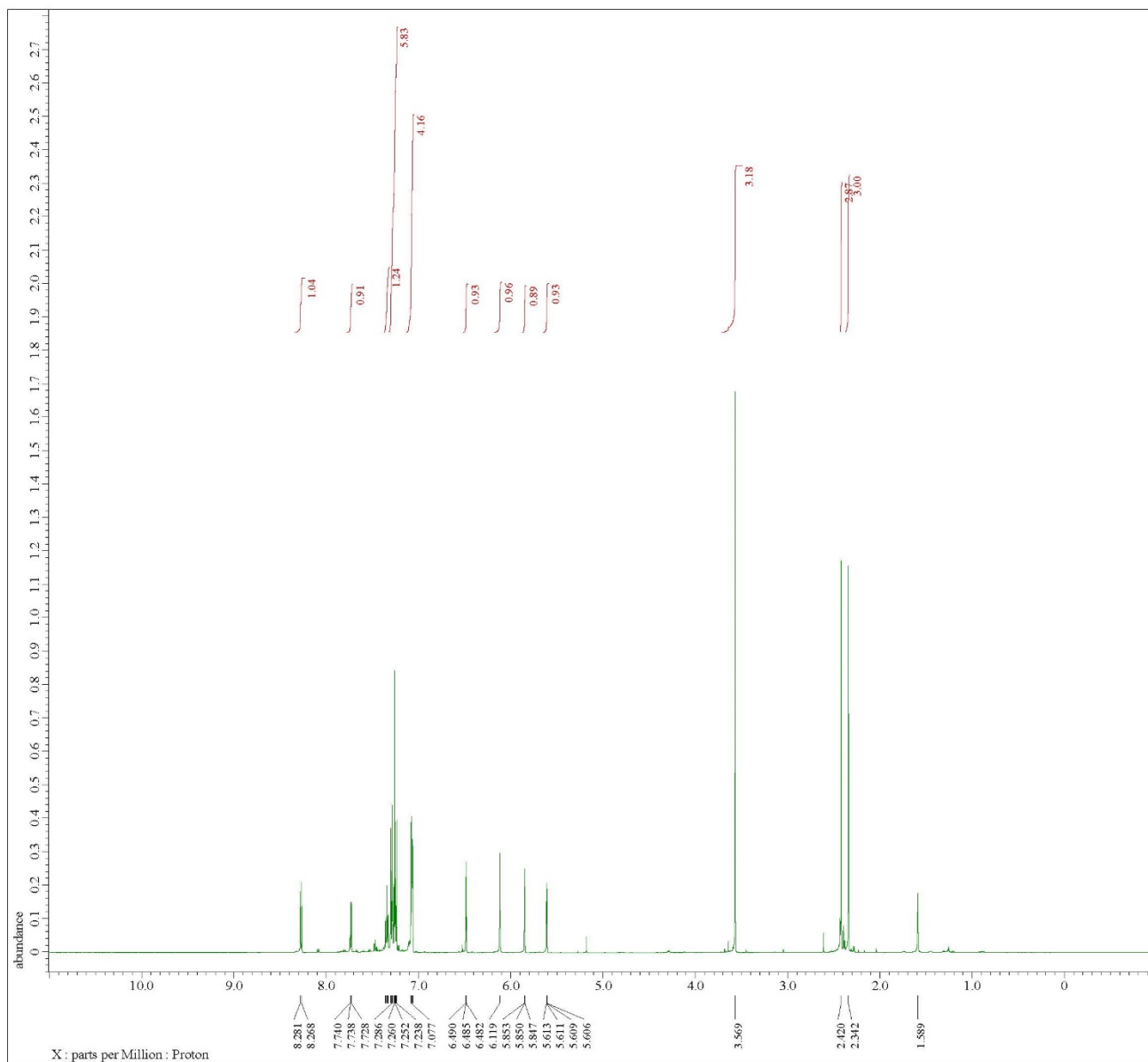
```



10d







```

---- PROCESSING PARAMETERS ----
smpc( 0.2[Hz], 0.0[F] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinphase
ppm
  
```

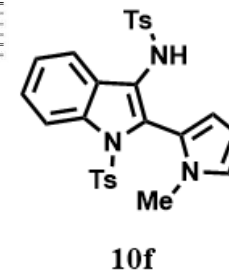
```

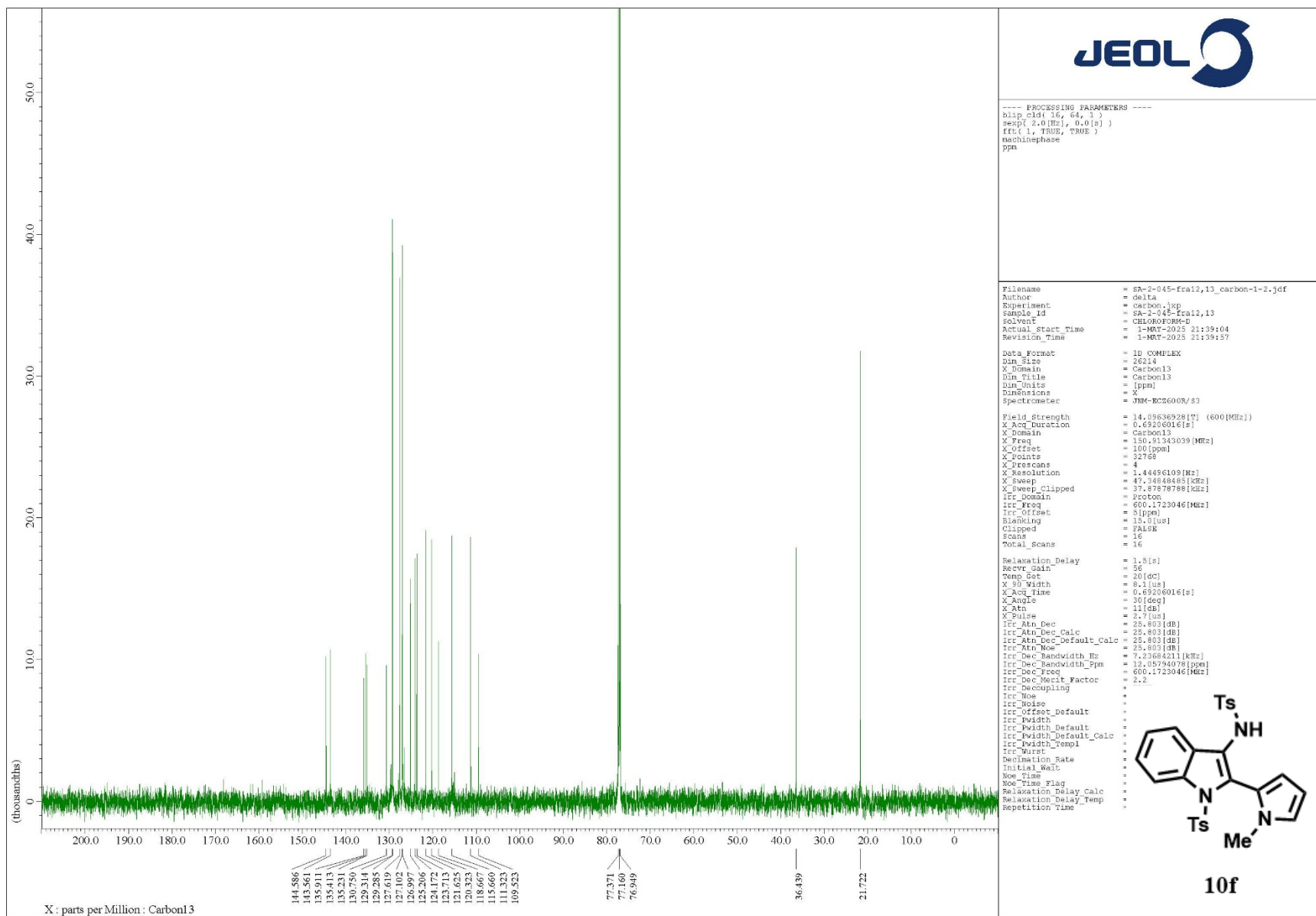
Filename      = SR-2-045-lower_proton-1-3.jdf
Author        = delta
Experiment    = proton.jpg
Sample_id     = SR-2-045-lower
Solvent       = CHLOROFORM-D
Actual_Start_Time = 8-MAY-2025 22:26:02
Revision_Time = 27-MAY-2025 11:28:31

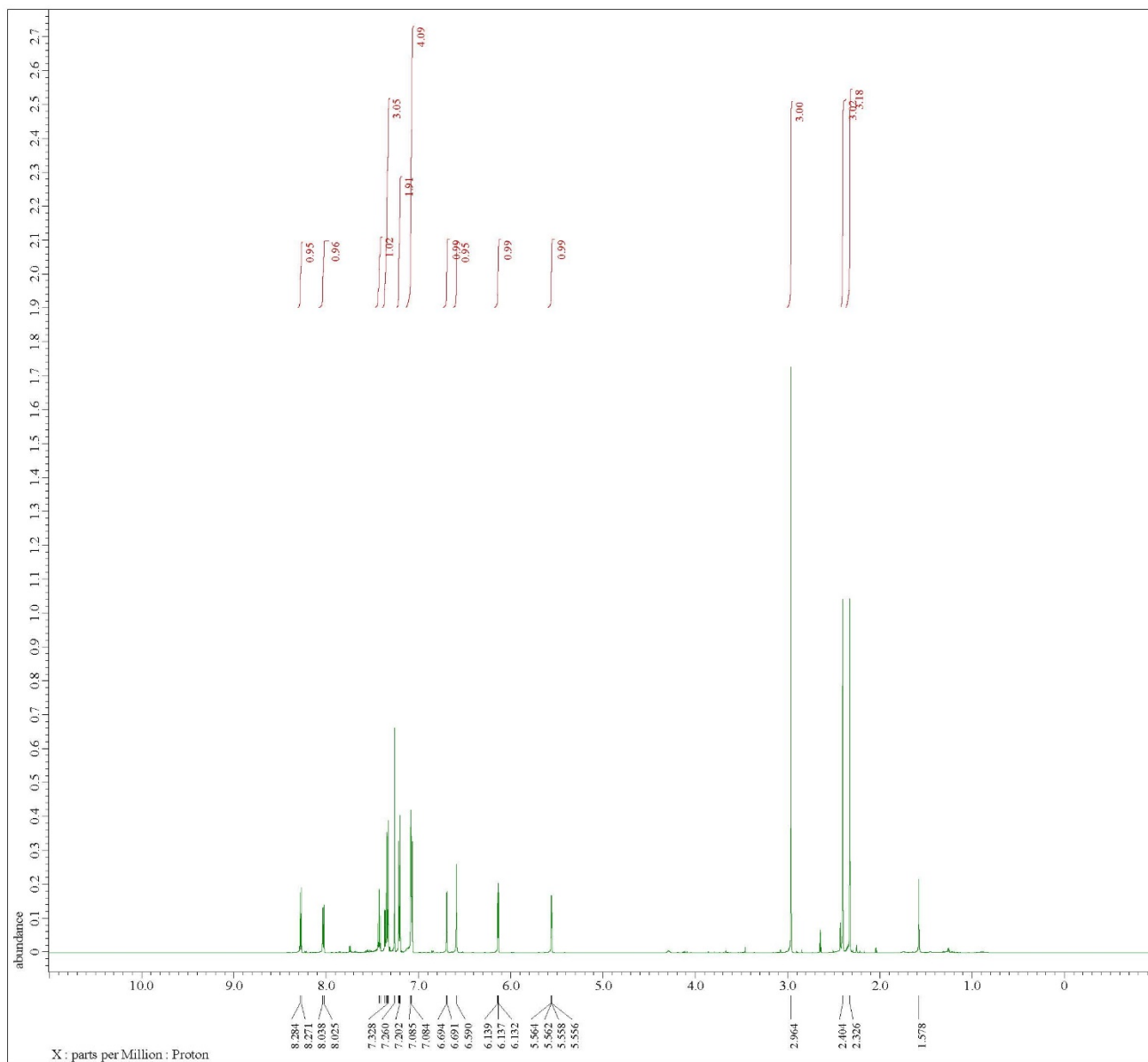
Data_Format   = 1D COMPLEX
Dim_Size      = 26214
X_Domain      = Proton
Dim_Title     = Proton
Dim_Units     = [ppm]
Dimensions    = 1
Spectrometer  = JNM-ECZ600R/S3

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  = 0.43849727[Hz]
X_Sweep       = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
f1c_Domain    = Proton
f1c_Freq      = 600.1723046[MHz]
f1c_Offset    = 5[ppm]
f1c_Domain    = Proton
f1c_Freq      = 600.1723046[MHz]
f1c_Offset    = 5[ppm]
Blanking      = 5.0[us]
Clipped       = FALSE
Scans         = 4
Total_Scans   = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 36
Temp_Set        = 21.7[degC]
X_90_Width      = 10.5[us]
X_Acq_Time      = 2.18103808[s]
X_Angle         = 45[deg]
X_Attn          = 8.1[dB]
X_Pulse         = 6.25[us]
TEC_Mode        = Off
TEC_Temp        = Off
Dante_Loop      = On
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase           =
Preset_Time     =
Preset_Time_Flag =
Relaxation_Delay_Calc =
Relaxation_Delay_Temp =
Repetition_Time =
  
```







```

---- PROCESSING PARAMETERS ----
sexpr( 0.2[Hz], 0.0[F] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinphase
ppm
  
```

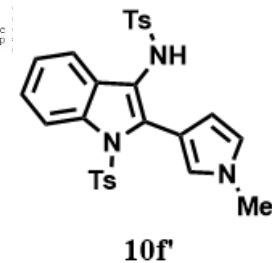
```

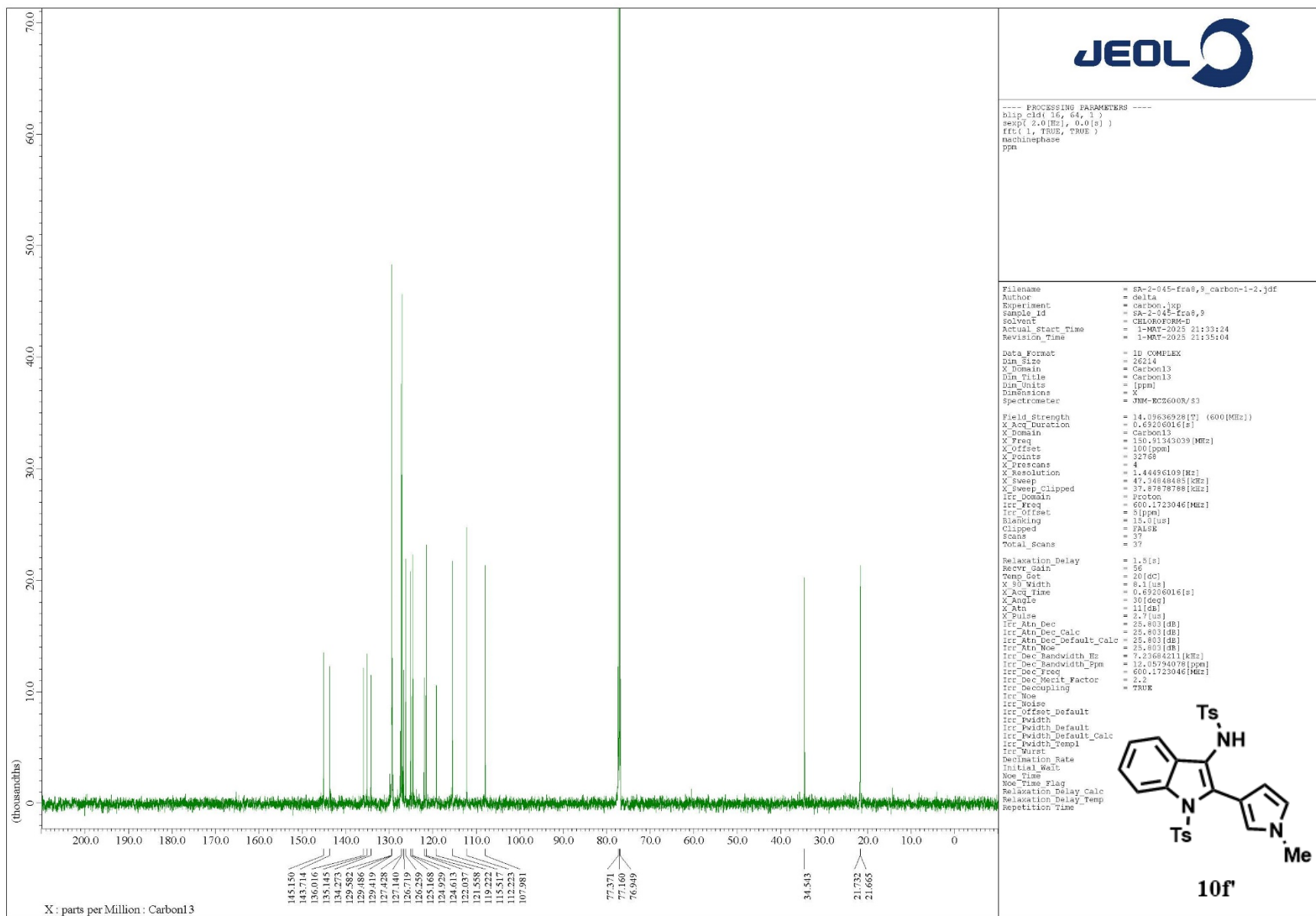
Filename      = SR-2-045-upper_proton-1-3.jdf
Author        = delta
Experiment    = proton_1xp
Sample_id     = SR-2-045-upper
Solvent       = CHLOROFORM-D
Actual_Start_Time = 8-MAY-2025 22:20:15
Revision_Time = 27-MAY-2025 11:27:36

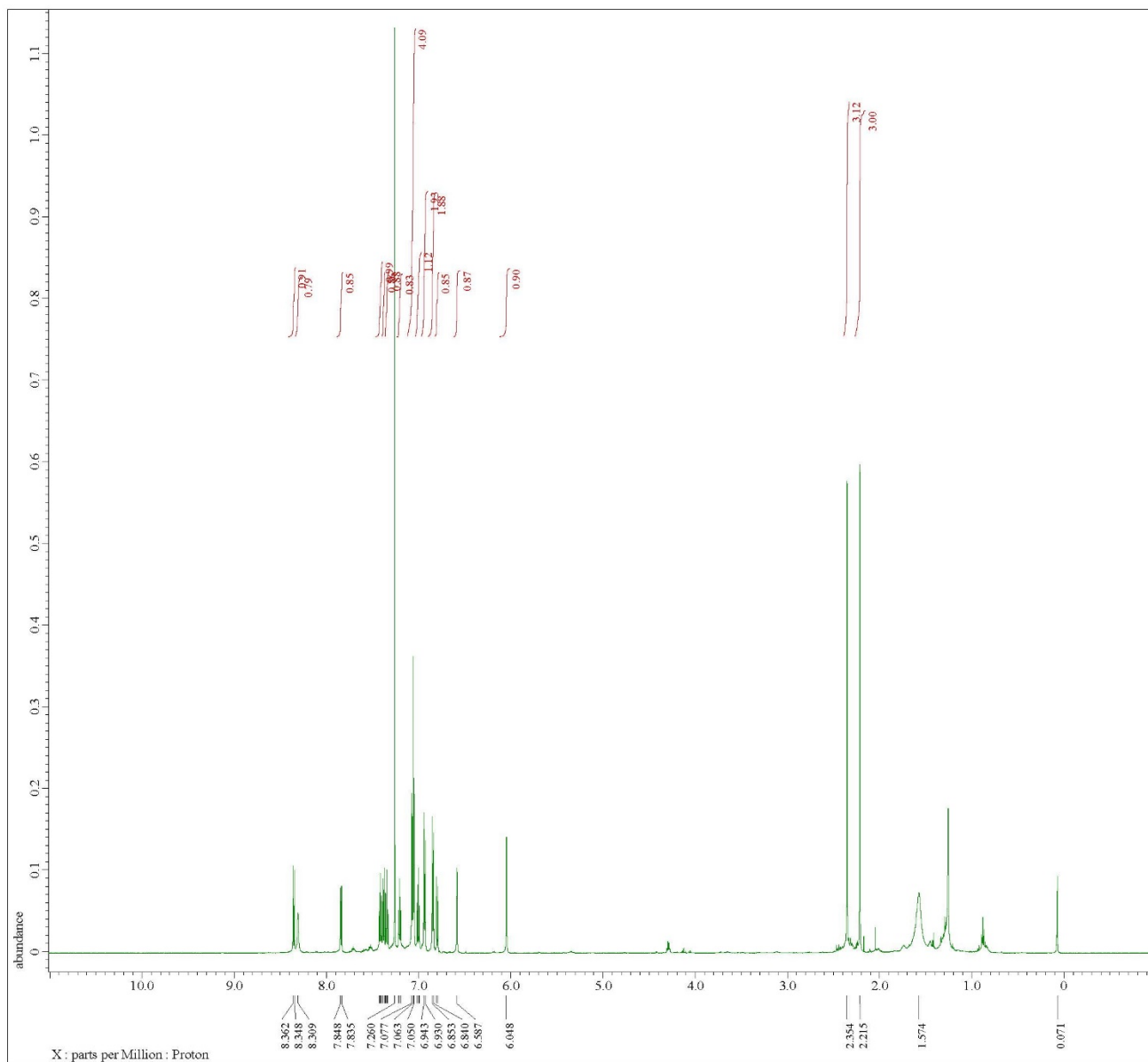
Data Format    = 1D COMPLEX
Bin Size      = 36214
X_Domain      = Proton
Din_Title     = Proton
Din_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-EC260R/S3

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_Clippped = 12.01923077[kHz]
F1r_Domain    = Proton
F1r_Freq      = 600.1723046[MHz]
F1r_Offset    = 5[ppm]
F2r_Domain    = Proton
F2r_Freq      = 600.1723046[MHz]
F2r_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[degC]
X_90_Width      = 10.5[us]
X_Acq Time      = 2.18103808[s]
X_Angle         = 45[deg]
X_Attn          = 8.1[dB]
X_Pulse         = 5.25[us]
TEr Mode        = Off
TEr Mode        = Off
Dante_Leap      = 200
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase           =
Preset_Time     =
Preset_Time_Flag =
Relaxation_Delay_Calc =
Relaxation_Delay_Temp =
Repetition_Time =
  
```







```

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

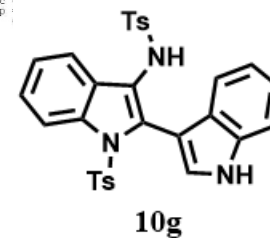
```

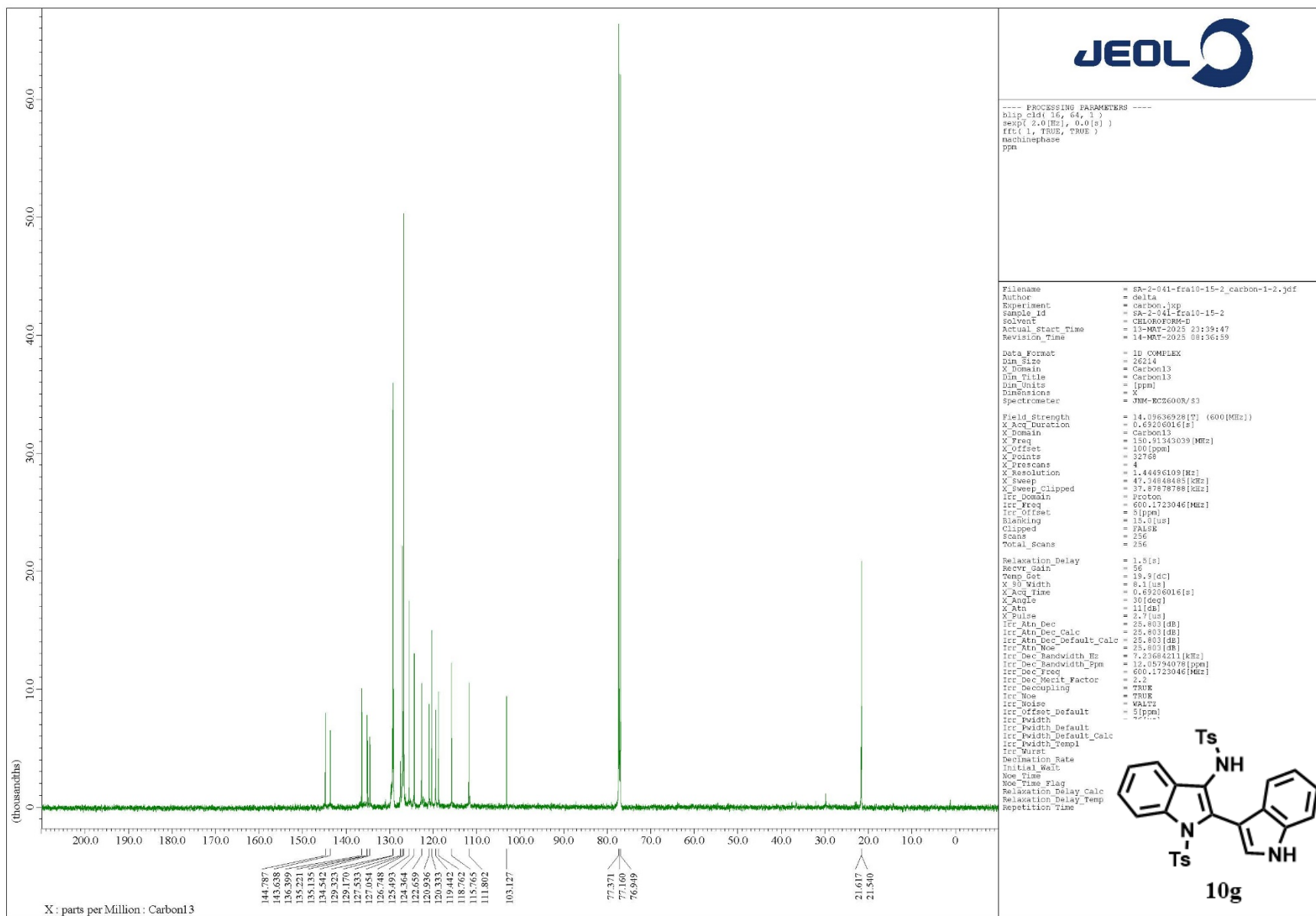
Filename      = SR-2-041-PTLC2_proton-1-3.jdf
Author       = delta
Experiment   = proton_1xp
Sample_id    = SR-2-041-PTLC2
Solvent      = CHLOROFORM-D
Actual_Start_Time = 25-MAY-2025 13:45:33
Revision_Time   = 27-MAY-2025 09:48:24

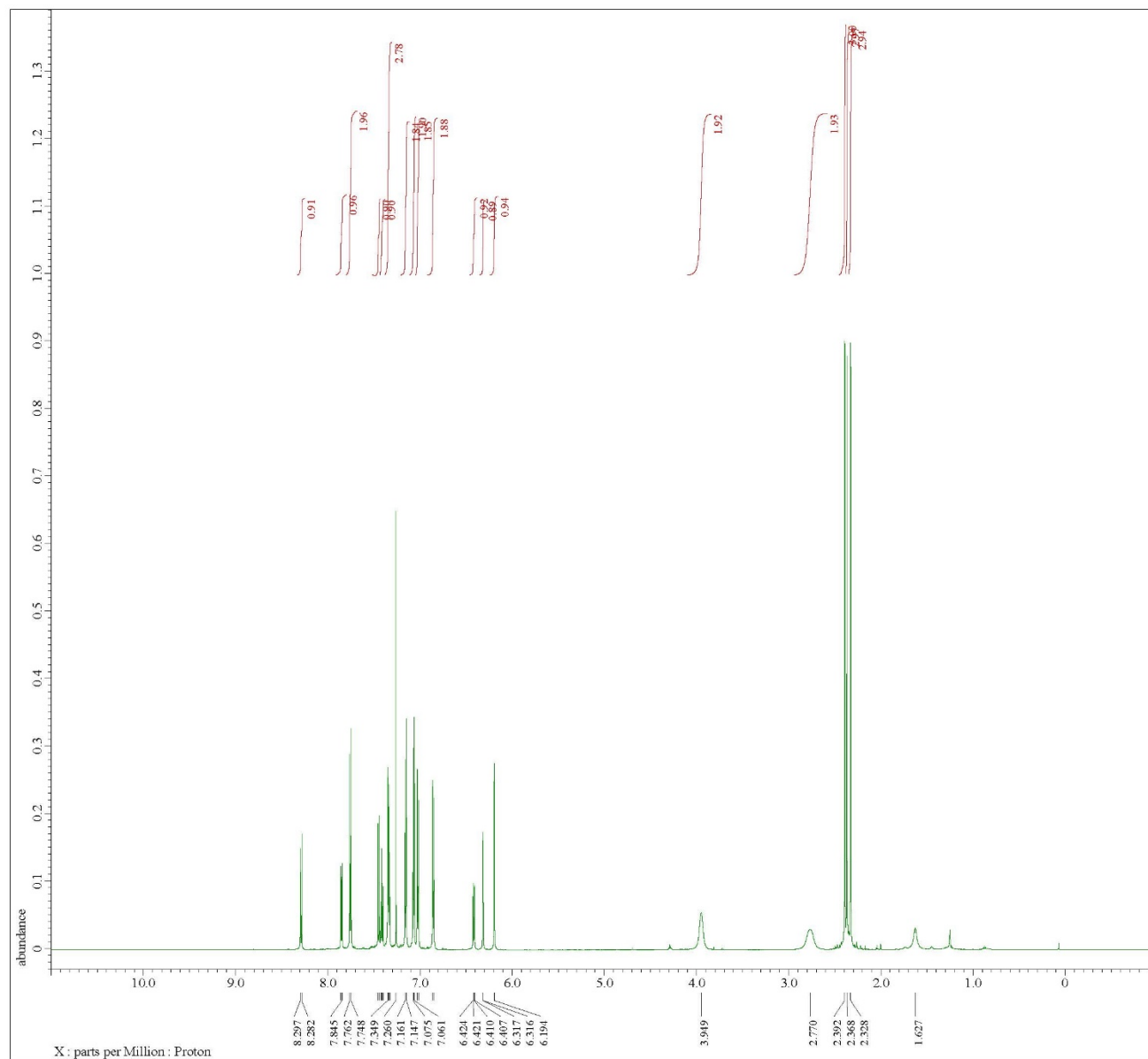
Data_Format   = 1D COMPLEX
Data_Size     = 26214
X_Domain      = Proton
Data_Title    = Proton
Data_Units    = [ppm]
Dimensions    = X
Spectrometer  = JNM-EC260R/S3

Field_Strength = 14.09636328[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   = 0.45049727[Hz]
X_Sweep        = 15.02403846[KHz]
X_Sweep_Clipped = 12.01923077[KHz]
F1r_Domain     = Proton
F1r_Freq       = 600.1723046[MHz]
F1r_Offset     = 5[ppm]
T1r_Domain     = Proton
T1r_Freq       = 600.1723046[MHz]
T1r_Offset     = 5[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 4
Total_Scans    = 4

Relaxation_Delay = 2[s]
Recvr_Gain       = 46
Temp_Set        = 26[degC]
X_90_Width      = 10.5[us]
X_Acq_Time      = 2.18103808[s]
X_Angle         = 45[deg]
X_Attn          = 8.1[dB]
X_Pulse         = 6.25[us]
F1r_Mode        = CFF
T1r_Mode        = CFF
Dante_Loop      = 200
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase           = [0, 90, 270, 180, 180, 270, 90, 0]
Preset_Time     = 2[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = ...
Relaxation_Delay_Temp = ...
Repetition_Time = ...
  
```







```

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

```

Filename      = SR-2-060-fra12-14_proton-2-3-jdf
Author       = delta
Experiment   = proton_1xp
Sample_id    = SR-2-060-fra12-14
Solvent      = CHLOROFORM-D
Actual_Start_Time = 20-MAY-2025 22:17:31
Revision_Time   = 27-MAY-2025 22:57:19

Data_Format   = 1D COMPLEX
Data_Size     = 26214
X_Domain      = Proton
Din_Title     = Proton
Din_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-EC260R/S3

Field_Strength = 14.09636328[T] (600[MHz])
X_Acq_Duration = 2.16103608[s]
X_Domain      = Proton
X_Freq        = 600.1723046[MHz]
X_Offset      = 5[ppm]
X_Points      = 32768
X_Prescans    = 1
X_Resolution  = 0.45049727[Hz]
X_Sweep       = 15.02403646[KHz]
X_Sweep_Clipped = 12.01923077[KHz]
F1r_Domain    = Proton
F1r_Freq      = 600.1723046[MHz]
F1r_Offset    = 5[ppm]
Tc1_Domain    = Proton
Tc1_Freq      = 600.1723046[MHz]
Tc1_Offset    = 5[ppm]
Blanking      = 5.0[us]
Clipped       = FALSE
Scans         = 8
Total_Scans   = 8

Relaxation_Delay = 2[s]
Recvr_Gain       = 36
Temp_Set        = 20.3[degC]
X_90_Width      = 10.5[us]
X_Acq_Time      = 2.16103608[s]
X_Angle         = 45[deg]
X_Attn          = 8.1[dB]
X_Pulse         = 6.25[us]
F1r_Mode        = CFF
Tc1_Mode        = CFF
Dante_Loop      = 200
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase          = [0, 90, 270, 180, 270, 90, 0]
Preset_Time     = 2[s]
Preset_Time_Flac = -----
Relaxation_Delay = -----
Relaxation_Delay = -----
Repetition_Time = -----
  
```

