Cis-3-Azido-2-Methoxyindolines as Safe and Stable Precursors to Overcome the Instability of Fleeting 3-Azidoindoles

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SUPPORTING INFORMATION

Contents

1. General Experimental

Melting points were recorded with a METTLER TOLEDO MP50 Melting Point System and are uncorrected. High-resolution MS spectra were recorded with a Brucker micrOTOF mass spectrometers (ESI-TOF-MS). IR spectra were measured with a Shimadzu IR Affinity-1 spectrometer. The NMR experiments were performed with JEOL JNM-ECZ600R (^{1}H NMR: 600 MHz, ^{13}C NMR: 151 MHz) spectrometer, and chemical shifts are expressed in ppm (δ) using residual undeuterated solvent as an internal reference ($CDCl_3$, ^{1}H NMR: δ 7.25, ^{13}C NMR: δ 77.1). The following abbreviations were used to explain NMR peak multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, sep = septet, m = multiplet, dd = doublet of doublets, ddd = doublet of doublet of doublets, dq = doublet of quartets, tt = triplet of triplets, br = broad; coupling constants in Hz; integration. The crystal structure of **3a** was determined by the single-crystal X-ray diffraction method at T = 103 K. The diffraction data was collected using Rigaku XtaLAB Synergy-i diffractometer (Cu–Kα radiation). The structure was solved using the SHELXT[S1] and refined with SHELXL-2018/3[S2] via OLEX2.[S3] All non-hydrogen atoms were refined anisotropically. All the hydrogen atoms were put on calculated geometrically, and were refined by applying riding models. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre: Deposition code CCDC 2107262 (**3a**).

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. Flash column chromatography was performed on silica gel (WAKO Gel 75−150 mesh, WAKO Co., Ltd.).

2. Experimental Procedure

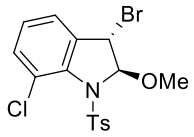
■Synthesis of *N*-protected indoles (1)

The *N*-protected indoles **1** as *N*-tosylindoles (**1a–1g**, **1l–1n**), *N*-benzenesulfonylindole (**1h**), *N*-(2-nitrobenzenesulfonyl)indole (**1i**), *N*-benzoylindole (**1j**) and *N*-acetylindole (**1k**) were prepared by reported methods.[S4–6] All substrates were used as received from commercial suppliers (Sigma-Aldrich, Kanto Chemical, TCI and Wako) and all reagents were weighed and handled in air at room temperature.

■General Procedure for the Bromoalkoxylation of 1

To a solution of *N*-protected indoles **1** (2.0 mmol) in MeOH (20 mL, 0.1 M) was added NBS (392 mg, 1.1 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material as indicated by TLC. After H_2O (20 mL) was added to the mixture, the whole was extracted with AcOEt (3 x 50 mL), washed with brine (25 mL). The combined organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by recrystallization from MeOH and/or silica gel column chromatography (AcOEt/hexane = 1/8–1/2) to give **2a**–**2k**. The other compounds (**2l, 2m** and **2n**) were prepared by our reported method.[S7]

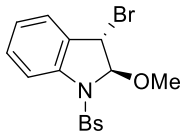
***trans*-3-Bromo-7-chloro-2-methoxy-1-tosylindoline (2g)**



2g

753 mg, 89% yield. colorless solid; mp 126–128 °C; IR (KBr): 1464, 1364, 1163, 1034, 991 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.66 (d, *J* = 7.8 Hz, 2H), 7.62 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.26–7.24 (m, 3H), 7.09 (t, *J* = 7.8 Hz, 1H), 5.90 (s, 1H), 4.87 (s, 1H), 3.49 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.5, 138.8, 136.5, 136.1, 132.6, 129.5, 128.2, 127.2, 125.0, 124.7, 101.0, 56.4, 45.9, 21.7; HRMS (ESI) *m/z*: 437.9544, 439.9516, 439.9522, 441.9492 (Calcd for $C_{16}H_{15}BrClNO_3SNa$ $[M+Na]^+$: 437.9542, 439.9513, 439.9522, 441.9492).

***trans*-1-Benzenesulfonyl-3-bromo-2-methoxyindoline (2h)**



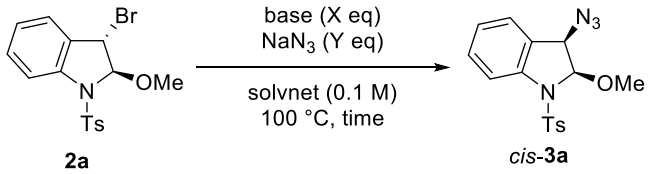
2h

671 mg, 91% yield. colorless solid; mp 108–110 °C; IR (KBr): 1468, 1354, 1169, 991 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.80–7.78 (m, 2H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.40–7.38 (m, 2H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 1H), 7.10 (t, *J* = 7.2 Hz, 1H), 5.56 (s, 1H), 4.92 (s, 1H), 3.60 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 140.5, 138.1, 133.7, 131.5, 130.7, 129.0, 127.7, 126.3, 125.6, 117.2, 99.9, 56.4, 47.1; HRMS (ESI) *m/z*: 389.9776, 391.9757 (Calcd for $C_{15}H_{14}BrNO_3SNa$ $[M+Na]^+$: 389.9776, 391.9755).

■Synthesis of 3-azido-2-alkoxyindolines (3a)

Optimization of Reaction Conditions

Table S1 Synthesis of 3-azido-2-methoxyindolines (3a)



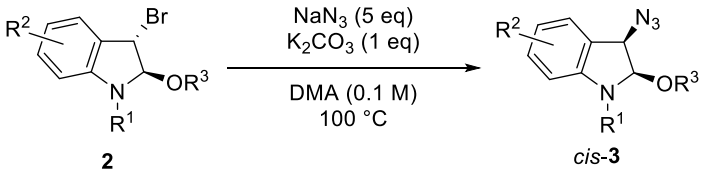
2a *cis*-**3a**

run	base (X eq)	NaN_3 (Y eq)	solvent	time (h)	yield (%)[a]
1	Et_3N (5)	5	DMF	1	74
2	Et_3N (5)	5	DMSO	1	85
3	Et_3N (5)	5	DMA	1	90
4	—	5	DMA	1	75
5	K_2CO_3 (5)	5	DMA	1	96
6	**K_2CO_3 (1)**	**5**	**DMA**	**1**	**95**
7	K_2CO_3 (0.5)	5	DMA	1	92
8	K_2CO_3 (5)	2	DMA	1	85
9	**K_2CO_3 (1)**	**5**	**DMA**	**0.5**	**95[b]**

[a] Isolated yields. [b] Stirred until the complete disapearance of starting material as indicated by TLC.

The solution of base (X mmol, X eq) and NaN_3 (Y mmol, Y eq) in solvent (10 mL, 0.1 M) was stirred at 100 °C in oil bath. To the mixture was added **2a** (382 mg, 1 mmol) and the mixture was stirred until the complete disappearance of starting material as indicated by TLC. After the reaction mixture was cooled down to room temperature, H_2O (10 mL) was added to the mixture. Then, the whole was extracted with AcOEt/hexane = 1/5 (3 x 25 mL), washed with H_2O (25 mL) and brine (25 mL). The combined organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/10–1/3) to give *cis*-**3a**.

■General Procedure for the synthesis of 3-azido-2-methoxyindolines 3 (Scheme 3)

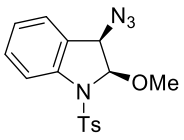


2 *cis*-**3**

To a solution of K_2CO_3 (138 mg, 1 mmol) and NaN_3 (325 mg, 5 mmol) in DMA (dimethylacetamide) (10 mL, 0.1 M) was added **2** (1 mmol) and the mixture was stirred at 100 °C in oil bath until the complete disappearance of starting material as indicated by TLC. After the reaction mixture was cooled down to room temperature, H_2O (10 mL) was added to the mixture. Then, the whole was extracted with AcOEt/hexane = 1/5 (3 x 25 mL), washed with H_2O (25 mL) and brine (25 mL). The combined organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by recrystallization from $CHCl_3$/hexane and/or silica gel column chromatography

(AcOEt/hexane = 1/10–1/3) to give *cis*-**3**.

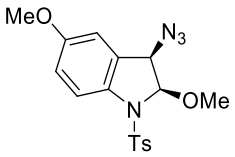
***cis*-3-Azido-2-methoxy-1-tosylindoline (3a)**



3a

Table S1, run 6: 326 mg, 95% yield. colorless solid; mp 97–100 °C; IR (KBr): 2106, 1464, 1348, 1167 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.57 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.32 (t, *J* = 8.4 Hz, 1H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.15 (t, *J* = 7.8 Hz, 1H), 5.40 (d, *J* = 6.0 Hz, 1H), 4.07 (d, *J* = 5.4 Hz, 1H), 3.62 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.6, 139.8, 135.8, 130.0, 130.0, 129.6, 126.9, 125.6, 124.4, 118.0, 95.6, 62.9, 56.8, 21.7; HRMS (ESI) *m/z*: 367.0839 (Calcd for $C_{16}H_{16}N_4O_3SNa$ $[M+Na]^+$: 367.0841).

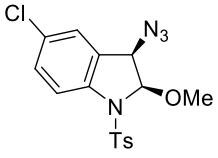
***cis*-3-Azido-2,5-dimethoxy-1-tosylindoline (3b)**



3b

321 mg, 85% yield. colorless solid; mp 132–134 °C; IR (KBr): 2118, 1489, 1350, 1167 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.53 (d, *J* = 9.0 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 6.86 (ddd, *J* = 8.4, 2.4, 0.6 Hz, 1H), 6.72 (dd, *J* = 2.4, 0.6 Hz, 1H), 5.33 (d, *J* = 5.4 Hz, 1H), 3.87 (d, *J* = 5.4 Hz, 1H), 3.78 (s, 3H), 3.61 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 158.3, 144.5, 135.6, 132.8, 131.8, 130.0, 126.8, 120.0, 115.1, 110.1, 95.1, 63.0, 56.4, 55.8, 21.7; HRMS (ESI) *m/z*: 397.0948 (Calcd for $C_{17}H_{18}N_4O_4SNa$ $[M+Na]^+$: 397.0947).

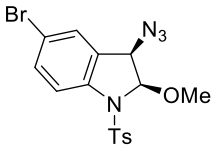
***cis*-3-Azido-5-chloro-2-methoxy-1-tosylindoline (3c)**



3c

377 mg, 99% yield. colorless solid; mp 101–103 °C; IR (KBr): 2118, 1468, 1360, 1167, 1105 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.55 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.29 (dd, *J* = 8.4, 0.6 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 1.2 Hz, 1H), 5.39 (d, *J* = 5.4 Hz, 1H), 4.02 (d, *J* = 5.4 Hz, 1H), 3.62 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.9, 138.4, 135.6, 131.7, 131.1, 130.1, 126.8, 124.7, 119.1, 94.8, 62.6, 56.8, 21.7; HRMS (ESI) *m/z*: 401.0451, 403.0422 (Calcd for $C_{16}H_{15}ClN_4O_3SNa$ $[M+Na]^+$: 401.0451, 403.0422).

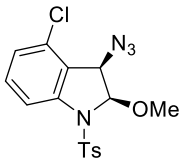
***cis*-3-Azido-5-bromo-2-methoxy-1-tosylindoline (3d)**



3d

333 mg, 79% yield. colorless solid; mp 111–112 °C; IR (KBr): 2116, 1466, 1364, 1167, 999 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.56 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 0.6 Hz, 1H), 7.44 (d, *J* = 0.6 Hz, 1H), 7.32 (dd, *J* = 2.4, 1.2 Hz, 1H), 7.21 (d, *J* = 7.2 Hz, 2H), 5.39 (d, *J* = 6.0 Hz, 1H), 4.05 (dd, *J* = 6.0, 1.2 Hz, 1H), 3.62 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.9, 138.9, 135.6, 133.1, 131.2, 130.1, 127.6, 126.8, 119.4, 118.5, 94.7, 62.5, 56.8, 21.7; HRMS (ESI) *m/z*: 444.9946, 446.9925 (Calcd for $C_{16}H_{15}BrN_4O_3SNa$ $[M+Na]^+$: 444.9946, 446.9926).

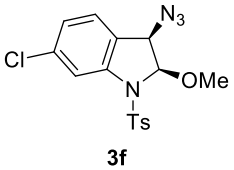
***cis*-3-Azido-4-chloro-2-methoxy-1-tosylindoline (3e)**



3e

360 mg, 95% yield. colorless oil; IR (KBr): 2112, 1466, 1362, 1171, 1005 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.66 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.27–7.23 (m, 3H), 7.09 (dd, *J* = 8.4, 1.2 Hz, 1H), 5.45 (d, *J* = 6.0 Hz, 1H), 4.30 (d, *J* = 6.0 Hz, 1H), 3.67 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.9, 141.9, 135.6, 131.7, 131.4, 130.1, 127.0, 126.1, 115.2, 94.0, 63.2, 57.3, 21.7; HRMS (ESI) *m/z*: 401.0450, 403.0422 (Calcd for $C_{16}H_{15}ClN_4O_3SNa$ $[M+Na]^+$: 401.0451, 403.0422).

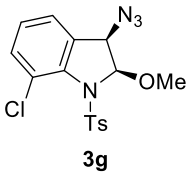
***cis*-3-Azido-6-chloro-2-methoxy-1-tosylindoline (3f)**



3f

345 mg, 91% yield. colorless solid; mp 129–128 °C; IR (KBr): 2114, 1474, 1350, 1169, 995 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.60 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 1.2 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.12–7.12 (m, 2H), 5.40 (d, *J* = 6.0 Hz, 1H), 4.06 (d, *J* = 5.4 Hz, 1H), 3.62 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.9, 141.0, 135.8, 135.7, 130.1, 128.0, 126.9, 125.6, 125.2, 118.1, 94.8, 62.4, 56.9, 21.7; HRMS (ESI) *m/z*: 401.0451, 403.0422 (Calcd for $C_{16}H_{15}ClN_4O_3SNa$ $[M+Na]^+$: 401.0451, 403.0422).

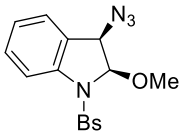
***cis*-3-Azido-7-chloro-2-methoxy-1-tosylindoline (3g)**



3g

371 mg, 98% yield. colorless solid; mp 120–122 °C; IR (KBr): 2112, 1464, 1364, 1173, 959 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.67 (ddd, *J* = 9.0, 1.8, 1.8 Hz, 2H), 7.40 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.27 (ddd, *J* = 9.0, 1.2, 1.2 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.15 (dd, *J* = 7.8, 1.2 Hz, 1H), 5.42 (d, *J* = 5.4 Hz, 1H), 4.07 (d, *J* = 5.4 Hz, 1H), 3.38 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.1, 138.0, 136.0, 135.5, 131.7, 130.0, 128.5, 128.4, 127.6, 122.6, 97.6, 63.3, 56.2, 21.8; HRMS (ESI) *m/z*: 401.0451, 403.0422 (Calcd for $C_{16}H_{15}ClN_4O_3SNa$ $[M+Na]^+$: 401.0451, 403.0422).

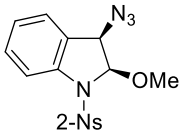
***cis*-3-Azido-1-benzenesulfonyl-2-methoxyindoline (3h)**



3h

290 mg, 88% yield. colorless solid; mp 129–131 °C; IR (KBr): 2120, 1464, 1354, 1169 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.70 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.53 (ddd, *J* = 7.8, 6.6, 1.2 Hz, 1H), 7.40 (ddd, *J* = 7.8, 6.0, 1.8 Hz, 2H), 7.33 (tt, *J* = 7.8, 1.2 Hz, 1H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.15 (ddd, *J* = 7.8, 1.2, 1.2 Hz, 1H), 5.42 (d, *J* = 5.4 Hz, 1H), 4.07 (d, *J* = 5.4 Hz, 1H), 3.63 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 139.7, 138.8, 133.6, 130.1, 129.5, 129.4, 126.8, 125.6, 124.5, 117.8, 94.6, 62.9, 56.8; HRMS (ESI) *m/z*: 353.0684 (Calcd for $C_{15}H_{14}N_4O_3SNa$ $[M+Na]^+$: 353.0684).

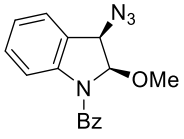
***cis*-3-Azido-2-methoxy-1-(2-nitrobenzenesulfonyl)indoline (3i)**



3i

30.6 mg, 8% yield. pale yellow solid; mp 116–117 °C; IR (KBr): 2116, 1474, 1346, 1167 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.08 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.53 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.28–7.27 (m, 2H), 7.22–7.17 (m, 3H), 7.07 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 5.88 (d, *J* = 6.0 Hz, 1H), 4.68 (d, *J* = 6.0 Hz, 1H), 3.67 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 138.9, 138.1, 134.9, 132.8, 129.9, 128.7, 128.6, 124.8, 124.8, 124.6, 120.0, 115.5, 95.4, 62.9, 56.9; HRMS (ESI) *m/z*: 398.0537 (Calcd for $C_{15}H_{13}N_5O_5SNa$ $[M+Na]^+$: 398.0535).

***cis*-3-Azido-1-benzoyl-2-methoxyindoline (3j)**

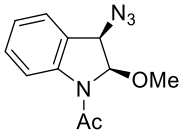


3j containing rotamers

220 mg, 75% yield. colorless crystal; mp 98–99 °C; IR (KBr): 2104, 1649, 1479, 1383 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.61 (d, *J* = 7.2 Hz, 2H), 7.56 (tt, *J* = 7.2, 1.8 Hz, 1H), 7.52–7.49 (m, 3H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.30 (br s, 1H), 7.21 (t, *J* = 7.2 Hz, 1H), 5.49 (br s, 1H), 4.75 (d, *J* = 5.4 Hz, 1H), 3.42 (s, 3H); ^{13}C NMR (151 MHz,

$CDCl_3$) δ: 170.0, 141.3, 135.9, 131.0, 129.7, 128.8, 128.0, 127.6, 124.9, 124.3, 117.7, 93.3, 62.6, 57.7; HRMS (ESI) *m/z*: 317.1015 (Calcd for $C_{16}H_{14}N_4O_2SNa$ $[M+Na]^+$: 317.1015).

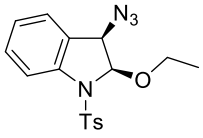
***cis*-1-Acetyl-3-azido-2-methoxyindoline (3k)**



3k containing rotamers

341 mg, 73% yield. yellow oil; IR (KBr): 2108, 1683, 1479, 1389 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.13 (d, *J* = 6.0 Hz, 1H), 7.41–7.27 (m, 2H), 7.10 (t, *J* = 7.2 Hz, 1H), 5.39 (s, 1H), 4.74 (s, 1H), 3.50 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 169.6, 141.6, 130.1, 126.4, 124.6, 124.1, 117.1, 91.5, 62.6, 56.4, 23.5; HRMS (ESI) *m/z*: 225.0858 (Calcd for $C_{11}H_{12}N_4O_2SNa$ $[M+Na]^+$: 225.0858).

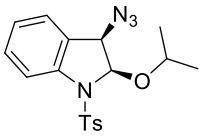
***cis*-3-Azido-2-ethoxy-1-tosylindoline (3l)**



3l

240 mg, 67% yield. colorless solid; mp 89–90 °C; IR (KBr): 2118, 1466, 1350, 1165 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.58 (ddd, *J* = 9.0, 1.8, 1.8 Hz, 2H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.32 (ddd, *J* = 7.8, 6.6, 1.2 Hz, 1H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.14 (ddd, *J* = 8.4, 7.8, 0.6 Hz, 1H), 5.50 (d, *J* = 6.0 Hz, 1H), 4.06 (d, *J* = 6.0 Hz, 1H), 4.30 (dq, *J* = 8.4, 7.2 Hz, 1H), 3.77 (dq, *J* = 8.4, 7.2 Hz, 1H), 2.35 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.5, 139.9, 136.0, 130.0, 129.9, 129.6, 126.9, 125.4, 124.4, 117.7, 93.2, 65.3, 62.8, 21.3, 15.0; HRMS (ESI) *m/z*: 381.0997 (Calcd for $C_{17}H_{18}N_4O_3SNa$ $[M+Na]^+$: 381.0997).

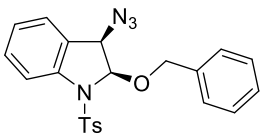
***cis*-3-Azido-2-isopropoxy-1-tosylindoline (3m)**



3m

362 mg, 97% yield. colorless solid; mp 107–109 °C; IR (KBr): 2118, 1466, 1350, 1165 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.55 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.53 (d, *J* = 9.0 Hz, 1H), 7.31 (ddd, *J* = 7.8, 6.0, 1.8 Hz, 1H), 7.21 (d, *J* = 7.8 Hz, 1H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.15 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 5.59 (d, *J* = 6.0 Hz, 1H), 4.31 (sep, *J* = 6.0 Hz, 1H), 3.97 (d, *J* = 5.4 Hz, 1H), 2.35 (s, 3H), 1.30 (d, *J* = 6.0 Hz, 3H), 1.20 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.4, 139.9, 136.1, 130.0, 129.9, 129.9, 126.8, 125.5, 124.4, 118.1, 91.5, 71.1, 62.7, 23.0, 21.6, 21.4; HRMS (ESI) *m/z*: 395.1154 (Calcd for $C_{18}H_{20}N_4O_3SNa$ $[M+Na]^+$: 395.1154).

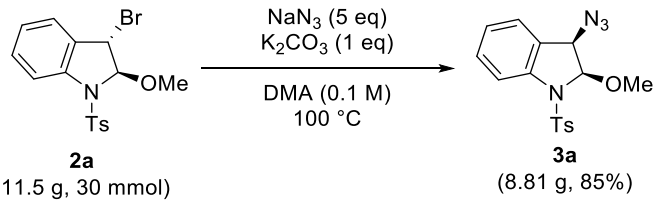
***cis*-3-Azido-2-benzyloxy-1-tosylindoline (3n)**



3n

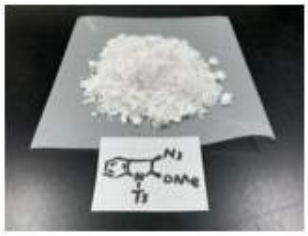
348 mg, 83% yield. colorless solid; mp 110–111 °C; IR (KBr): 2104, 1462, 1364, 1173 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.59 (d, *J* = 7.8 Hz, 1H), 7.51 (ddd, *J* = 7.8, 1.8, 1.8 Hz, 2H), 7.40 (d, *J* = 7.2 Hz, 2H), 7.35–7.32 (m, 3H), 7.29 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.16 (t, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 7.8 Hz, 2H), 5.57 (d, *J* = 5.4 Hz, 1H), 5.00 (d, *J* = 12.0 Hz, 1H), 4.86 (d, *J* = 12.0 Hz, 1H), 4.03 (d, *J* = 5.4 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.6, 139.9, 137.0, 135.8, 130.1, 130.0, 129.7, 128.5, 128.0, 127.9, 126.8, 125.7, 124.4, 118.2, 92.6, 70.7, 63.0, 21.6; HRMS (ESI) *m/z*: 443.1154 (Calcd for $C_{22}H_{20}N_4O_3SNa$ $[M+Na]^+$: 443.1154).

■Gram-scale synthesis of 3-azido-2-methoxy-1-tosylindoline (3a)



2a
(11.5 g, 30 mmol)

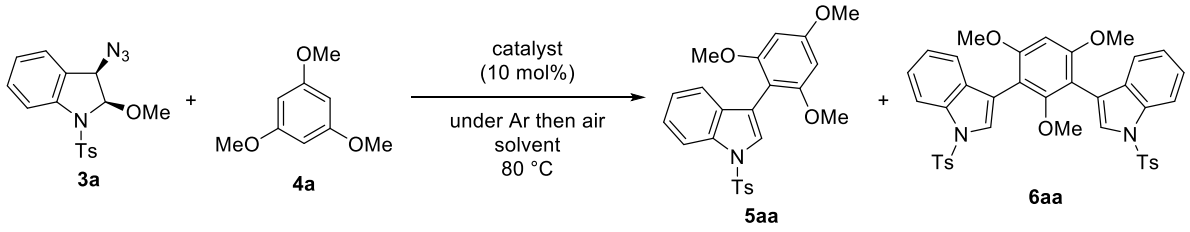
3a
(8.81 g, 85%)



A solution of K_2CO_3 (4.16 g, 30 mmol) and NaN_3 (9.75 g, 150 mmol) in DMA (dimethylacetamide) (300 mL, 0.1 M) was stirred at 100 °C in oil bath. To the mixture was added **2a** (11.5 g, 30 mmol) and stirred for 1 h at 100 °C. After the reaction mixture was cooled down to room temperature, H_2O (50 mL) was added to the mixture. Then, the whole was extracted with AcOEt/hexane = 1/5 (3 x 100 mL), washed with H_2O (100 mL) and brine (100 mL). The combined organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by recrystallization from $CHCl_3$/hexane to give **3a** (8.81g, 85%).

Optimization of Reaction Conditions

Table S2 Optimization of reaction conditions using 3a and 4a

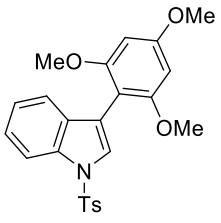


run	cat. (10 mol%)	solvent (mL)	time (h)	yield (%)	
				5aa[a]	**6aa**[a]
1	$In(OTf)_3$	DCE (3)	2	18	8
2	$InF_3•4H_2O$	DCE (3)	2	trace	0
3	$InBr_3$	DCE (3)	1	74	15
4	**$InCl_3•4H_2O$**	**DCE (3)**	**1**	**77**	**17**
5	$AlCl_3$	DCE (3)	2	42	3
6	$LaCl_3•7H_2O$	DCE (3)	2	trace	0
7	$FeCl_3$	DCE (3)	1	73	20
8	$BF_3•OEt_2$	DCE (3)	1	67	6
9	$InCl_3•4H_2O$	toluene (3)	2	48	0
10	$InCl_3•4H_2O$	ClC_6H_5 (3)	2	54	3
11	$InCl_3•4H_2O$	$CF_3C_6H_5$ (3)	2	67	13
12	$InCl_3•4H_2O$	HFIP (3)	1	72	8
13	$InCl_3•4H_2O$	MeOH (3)	2	nr	nr
14	$InCl_3•4H_2O$	DCE (3)	1	21	58
15	—	DCE (3)	16	nr	nr
16[c]	**$InCl_3•4H_2O$**	**DCE (1.5)**	**0.5**	**77**	**17**
17	$InCl_3•4H_2O$	DCE (0.6)	1	76	14

[a] Isolated yields. [b] **3a** (0.3 mmol), and **4a** (0.15 mmol), and $InCl_3•4H_2O$ (0.03 mmol) in DCE (3 mL).

To a solution of **3a** (103 mg, 0.3 mmol) and 1,3,5-trimethoxybenzene **4a** (55.5 mg, 0.33 mmol) in solvent (3 mL, 0.1 M) was added catalyst (0.03 mmol) under Ar. The mixture was stirred at 80 °C in oil bath until the complete disappearance of starting material and 3-azidoindole as indicated by TLC or for 2 h. After H_2O (0.1 mL) was added to the mixture at 80 °C, and the mixture was stirred at 80 °C for 30 min. The whole was cooled to room temperature and H_2O (10 mL) was added to the mixture. Then, the whole was extracted with $CHCl_3$ (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/10–1/2) to give **5aa** and **6aa**.

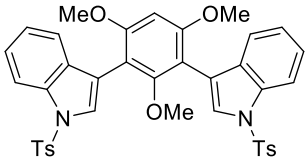
1-Tosyl-3-(2,4,6-trimethoxyphenyl)indole (5aa)



5aa

Table S2, run 4: 101 mg, 77% yield. colorless solid; mp 122–123 °C; IR (KBr): 1454, 1364, 1179, 1125 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.97 (d, *J* = 8.4 Hz, 1H), 7.62 (ddd, *J* = 8.4, 1.2, 1.2 Hz, 2H), 7.59 (s, 1H), 7.24 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 2H), 7.14 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 6.23 (s, 2H), 3.89 (s, 3H), 3.69 (s, 6H), 2.32 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.2, 159.2, 144.7, 135.6, 134.9, 131.5, 129.8, 1267.0, 126.5, 124.0, 122.9, 121.7, 115.3, 113.5, 102.7, 91.0, 55.8, 55.5, 21.7; HRMS (ESI) *m/z*: 460.1195 (Calcd for $C_{24}H_{23}NO_5SNa$ $[M+Na]^+$: 460.1195).

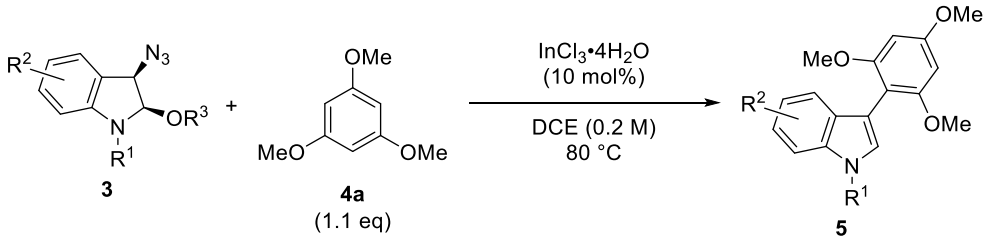
3,3'-(2,4,6-trimethoxy-1,3-phenylene)bis-1-tosylindole (6aa)



6aa

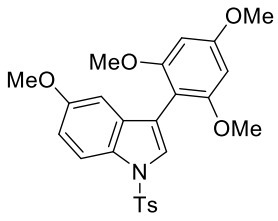
Table S2, run 4: 17.8 mg, 17% yield. colorless solid; mp 229–231 °C; IR (KBr): 1445, 1366, 1175, 1109 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.00 (d, *J* = 7.8 Hz, 2H), 7.77 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 4H), 7.64 (s, 2H), 7.36 (d, *J* = 7.8 Hz, 2H), 7.29 (ddd, *J* = 7.8, 6.6, 1.2 Hz, 2H), 7.20 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 2H), 7.17 (d, *J* = 7.8 Hz, 4H), 6.46 (s, 1H), 3.77 (s, 6H), 2.72 (s, 3H), 2.30 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 159.0, 158.8, 144.8, 135.5, 135.0, 131.3, 129.8, 126.9, 126.1, 124.4, 123.2, 121.6, 115.7, 113.6, 107.9, 91.9, 60.5, 55.9, 21.6; HRMS (ESI) *m/z*: 729.1706 (Calcd for $C_{39}H_{34}N_2O_7S_2Na$ $[M+Na]^+$: 729.1705).

■General Procedure for the reaction of 3 with 4a (Scheme 4)



To a solution of **3** (0.3 mmol) and **4a** (55.5 mg, 0.33 mmol) in 1,2-dichloroethane (DCE) (1.5 mL, 0.2 M) was added $InCl_3$•$4H_2O$ (8.8 mg, 0.03 mmol) under Ar. The mixture was stirred at 80 °C in oil bath until the complete disappearance of starting material and 3-azidoindole as indicated by TLC or for 24 h. After H_2O (0.1 mL) was added to the mixture at 80 °C, and the mixture was stirred at 80 °C for 30 min. The mixture was then allowed to cool to room temperature and was diluted with H_2O (10 mL). Then, the whole was extracted with $CHCl_3$ (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/10–1/3) to give **5ba–5ka**.

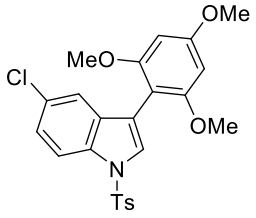
5-Methoxy-1-tosyl-3-(2,4,6-trimethoxyphenyl)indole (5ba)



5ba

118 mg, 84% yield. colorless solid; mp 107–109 °C; IR (KBr): 1472, 1364, 1173, 1126 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.85 (d, *J* = 9.0 Hz, 1H), 7.75 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.55 (s, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.86 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.66 (d, *J* = 3.0 Hz, 1H), 6.23 (s, 2H), 3.87 (s, 3H), 3.71 (s, 3H), 3.70 (s, 6H), 2.32 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.2, 159.2, 156.2, 144.5, 135.6, 132.6, 129.7, 127.4, 126.9, 115.5, 114.4, 113.2, 104.1, 102.8, 91.0, 55.8, 55.7, 55.5, 21.6; HRMS (ESI) *m/z*: 490.1300 (Calcd for $C_{25}H_{25}NO_6SNa$ $[M+Na]^+$: 490.1300).

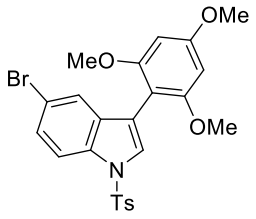
5-Chloro-1-tosyl-3-(2,4,6-trimethoxyphenyl)indole (5ca)



5ca

111 mg, 79% yield. colorless solid; mp 142–143 °C; IR (KBr): 1468, 1371, 1175, 1126, 1009 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.88 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.50 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.59 (s, 1H), 7.22–7.19 (m, 4H), 6.22 (s, 2H), 3.87 (s, 3H), 3.70 (s, 6H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.5, 159.1, 144.9, 135.3, 133.3, 132.9, 129.9, 128.8, 127.8, 126.9, 124.2, 121.4, 114.9, 114.6, 102.0, 91.0, 55.8, 55.5, 21.7; HRMS (ESI) *m/z*: 494.0806, 496.0775 (Calcd for $C_{24}H_{22}ClNO_5SNa$ $[M+Na]^+$: 494.0805, 496.0775).

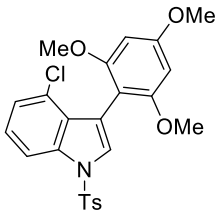
5-Bromo-1-tosyl-3-(2,4,6-trimethoxyphenyl)indole (5da)



5da

118 mg, 76% yield. colorless solid; mp 153–154 °C; IR (KBr): 1456, 1371, 1175, 1125, 1009 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.83 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 9.0 Hz, 2H), 7.57 (s, 1H), 7.35–7.32 (m, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 6.22 (s, 2H), 3.87 (s, 3H), 3.70 (s, 6H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.5, 159.1, 145.0, 135.3, 133.7, 133.3, 129.9, 127.6, 126.9, 126.8, 124.5, 116.6, 115.0, 114.8, 102.0, 91.0, 55.8, 55.5, 21.7; HRMS (ESI) *m/z*: 538.0300, 540.0279 (Calcd for $C_{24}H_{22}BrNO_5SNa$ $[M+Na]^+$: 538.0300. 540.0279).

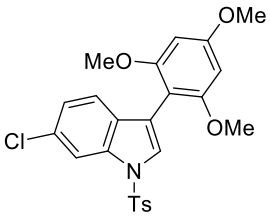
4-Chloro-1-tosyl-3-(2,4,6-trimethoxyphenyl)indole (5ea)



5ea

109 mg, 77% yield. colorless solid; mp 166–168°C; IR (KBr): 1456, 1377, 1175, 1132, 1024 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.88 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.75 (ddd, *J* = 6.6, 1.8, 1.8 Hz, 2H), 7.49 (s, 1H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.14 (t, *J* = 3.6 Hz, 1H), 7.09 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.17 (s, 2H), 3.86 (s, 3H), 3.66 (s, 6H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.5, 159.7, 145.0, 136.4, 135.3, 129.9, 128.6, 127.4, 127.2, 127.0, 124.6, 124.4, 114.9, 112.3, 103.2, 90.5, 55.8, 55.4, 21.7; HRMS (ESI) *m/z*: 494.0805, 496.0776 (Calcd for $C_{24}H_{22}ClNO_5SNa$ $[M+Na]^+$: 494.0805, 496.0775).

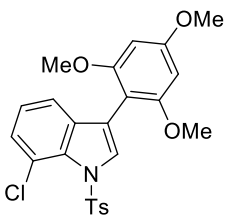
6-Chloro-1-tosyl-3-(2,4,6-trimethoxyphenyl)indole (5fa)



5fa

103 mg, 73% yield. colorless oil; IR (KBr): 1456, 1371, 1177, 1128, 1011 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.99 (d, *J* = 1.2 Hz, 1H), 7.62 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.57 (s, 1H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.15 (d, *J* = 7.8 Hz, 1H), 7.12 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.22 (s, 2H), 3.86 (s, 3H), 3.69 (s, 6H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.4, 159.1, 145.0, 135.4, 135.2, 130.0, 129.9, 127.0, 126.9, 123.5, 122.6, 115.1, 113.7, 102.2, 91.0, 55.8, 55.5, 21.7; HRMS (ESI) *m/z*: 494.0804, 496.0776 (Calcd for $C_{24}H_{22}ClNO_5SNa$ $[M+Na]^+$: 494.0805, 496.0775).

7-Chloro-1-tosyl-3-(2,4,6-trimethoxyphenyl)indole (5ga)

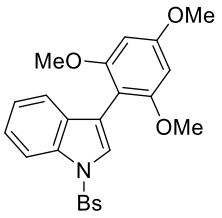


5ga

49.0 mg, 35% yield. colorless solid; mp 173–175 °C; IR (KBr): 1458, 1362, 1177, 1128, 1003 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 7.86 (s, 1H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.16 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.13 (dd, *J* = 7.8, 0.6 Hz, 1H), 7.03 (t, *J* = 1.8 Hz, 1H), 6.24 (s, 2H), 3.88 (s, 3H), 3.72 (s, 6H), 2.38 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.5, 159.4, 144.4, 137.4, 135.4, 131.9, 130.3, 129.7, 127.3, 126.3, 123.7, 120.1, 118.9, 113.8,

102.1, 90.9, 55.9, 55.5, 21.7; HRMS (ESI) *m/z*: 494.0806, 496.0774 (Calcd for $C_{24}H_{22}ClNO_5SNa$ $[M+Na]^+$: 494.0805, 496.0775).

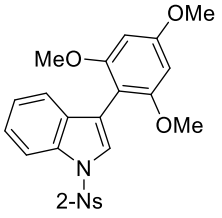
1-Bezenesulfonyl-3-(2,4,6-trimethoxyphenyl)indole (5ha)



5ha

101 mg, 80% yield. colorless solid; mp 96–98 °C; IR (KBr): 1447, 1364, 1182, 1128 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.01 (d, *J* = 8.4 Hz, 1H), 7.90 (ddd, *J* = 7.2, 1.8, 1.8 Hz, 2H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.40 (s, 1H), 7.38 (ddd, *J* = 7.2, 1.8, 1.8 Hz, 2H), 7.27 (ddd, *J* = 7.8, 6.6, 0.6 Hz, 1H), 7.26 (d, *J* = 7.8 Hz, 1H), 7.17 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 6.25 (s, 2H), 3.87 (s, 3H), 3.68 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.3, 159.2, 138.5, 135.0, 133.6, 131.6, 129.2, 126.9, 126.4, 124.1, 123.0, 121.8, 115.7, 113.6, 102.7, 91.1, 55.8, 55.5; HRMS (ESI) *m/z*: 446.1037 (Calcd for $C_{23}H_{21}NO_5SNa$ $[M+Na]^+$: 446.1038).

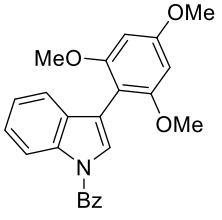
1-(2-Nitrobenzenesulfonyl)-3-(2,4,6-trimethoxyphenyl)indole (5ia)



5ia

0.05 mmol scale: 18.8 mg, 80% yield. colorless solid; mp 171–173 °C; IR (KBr): 1578, 1466, 1371, 1180, 1016 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.14 (d, *J* = 8.4 Hz, 1H), 7.77 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.55 (t, *J* = 8.4 Hz, 1H), 7.27–7.24 (m, 2H), 7.19–7.13 (m, 3H), 6.25 (s, 2H), 3.88 (s, 3H), 3.72 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 161.2, 159.4, 139.2, 135.0, 134.3, 131.4, 131.0, 129.1, 127.8, 124.6, 123.6, 122.7, 121.6, 120.2, 113.3, 112.8, 102.7, 90.9, 55.9, 55.5; HRMS (ESI) *m/z*: 491.0892 (Calcd for $C_{23}H_{20}N_2O_7SNa$ $[M+Na]^+$: 491.0889).

1-Benzoyl-3-(2,4,6-trimethoxyphenyl)indole (5ja)

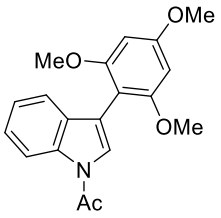


5ja

71.0 mg, 61% yield. colorless solid; mp 138–139 °C; IR (KBr): 1678, 1450, 1368, 1126 cm^{-1}; ^1H NMR (600 MHz,

$CDCl_3$) δ: 8.45 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 7.2 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.37 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.33 (s, 1H), 7.33 (d, *J* = 6.0 Hz, 1H), 7.27 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 6.24 (s, 2H), 3.87 (s, 3H), 3.72 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 168.6, 161.2, 159.3, 136.1, 135.1, 131.7, 131.4, 129.4, 128.5, 127.5, 124.5, 123.6, 121.1, 116.4, 114.7, 103.0, 91.0, 55.9, 55.5; HRMS (ESI) *m/z*: 410.1368 (Calcd for $C_{24}H_{21}NO_4SNa$ $[M+Na]^+$: 410.1368).

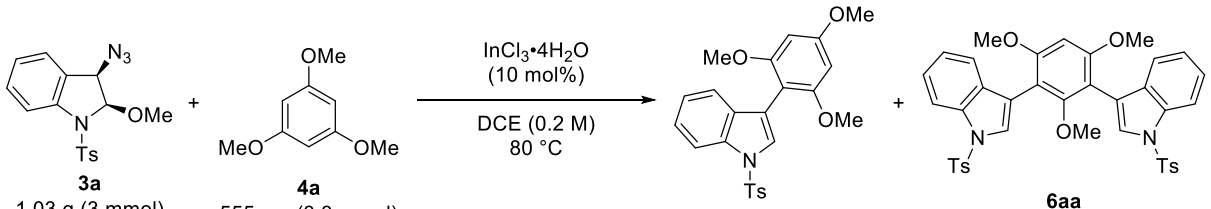
1-Acetyl-3-(2,4,6-trimethoxyphenyl)indole (5ka)



5ka

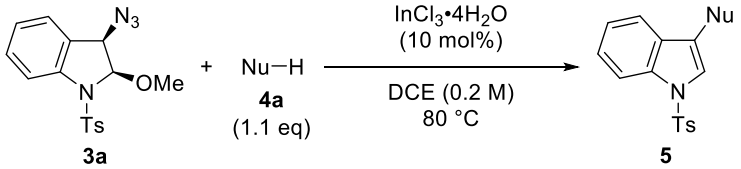
14.5 mg, 15% yield. colorless solid; mp 142–144 °C; IR (KBr): 1717, 1456, 1339, 1125 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.45 (d, *J* = 8.4 Hz, 1H), 7.41 (s, 1H), 7.31 (ddd, *J* = 8.4, 7.8, 0.6 Hz, 1H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.20 (t, *J* = 7.2 Hz, 1H), 6.27 (s, 2H), 3.88 (s, 3H), 3.72 (s, 6H), 2.63 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 168.4, 161.3, 159.5, 135.7, 131.2, 125.0, 124.6, 123.2, 120.9, 116.5, 115.4, 103.3, 91.4, 55.9, 55.5, 24.0; HRMS (ESI) *m/z*: 348.1212 (Calcd for $C_{19}H_{19}NO_4SNa$ $[M+Na]^+$: 348.1212).

■Gram-scale synthesis of 5aa and 6aa



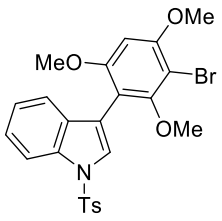
To a solution of **3a** (1.03 g, 3 mmol) and **4a** (555 mg, 3.3 mmol) in DCE (15 mL, 0.2 M) was added $InCl_3$•$4H_2O$ (87.9 mg, 0.3 mmol). The mixture was stirred at 80 °C in oil bath for 1 h. After H_2O (1 mL) was added to the mixture at 80 °C, and the mixture was stirred at 80 °C for 30 min. The reaction mixture was cooled to room temperature and diluted with H_2O (15 mL). Then, the whole was extracted with $CHCl_3$ (3 x 50 mL), washed with brine (50 mL). The combined organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/10–1/2) to give **5aa** (981 mg, 75%) and **6aa** (171 mg, 16%).

■General Procedure for the synthesis of 5



To a solution of **3a** (344 mg, 1 mmol) and nucleophiles **4** (1.1 mmol) in DCE (5 mmol, 0.2 M) was added $InCl_3$•$4H_2O$ (29.3 mg, 0.1 mmol) under Ar. The mixture was stirred at 80 °C in oil bath until the complete disappearance of starting material and 3-azidoindole as indicated by TLC or for 24 h. After H_2O (1 mL) was added to the mixture at 80 °C, and the mixture was stirred at 80 °C for 30 min. The reaction mixture was cooled to room temperature and H_2O (10 mL) was added to the mixture. Then, the whole was extracted with $CHCl_3$ (3 x 25 mL), washed with brine (25 mL). The organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/10–1/1, and/or toluene/hexane = 1/2–1/1) to give **5**.
Nucleophiles **4b**, **4c** and **4d** were prepared by reported methods.[S8–10] The other nucleophiles were used as received from commercial suppliers (Sigma-Aldrich, Kanto Chemical, TCI and Wako).

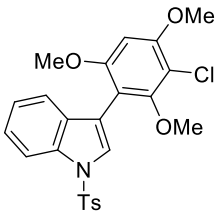
3-(3-bromo-2,4,6-trimethoxyphenyl)-1-tosylindole (5ab)



5ab

275 mg, 53% yield. colorless solid; mp 145–146 °C; IR (KBr): 1449, 1369, 1177, 1115, 1016 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.03 (d, *J* = 8.4 Hz, 1H), 7.78 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.64 (s, 1H), 7.30 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.21–7.17 (m, 3H), 6.42 (s, 1H), 3.96 (s, 3H), 3.72 (s, 3H), 3.23 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 158.4, 157.2, 157.1, 144.9, 135.5, 135.0, 130.9, 129.8, 126.9, 126.3, 124.5, 123.2, 121.5, 115.2, 113.7, 109.1, 98.7, 92.8, 60.4, 56.6, 56.1, 21.6; HRMS (ESI) *m/z*: 538.0301, 540.0280 (Calcd for $C_{24}H_{22}BrNO_5SNa$ $[M+Na]^+$: 538.0300. 540.0279).

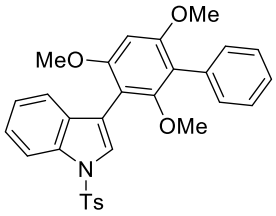
3-(3-chloro-2,4,6-trimethoxyphenyl)-1-tosylindole (5ac)



5ac

324 mg, 69% yield. colorless solid; mp 158–160 °C; IR (KBr): 1450, 1379, 1177, 1119, 1018 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.03 (d, *J* = 7.8 Hz, 1H), 7.78 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.63 (s, 1H), 7.29 (ddd, *J* = 9.0, 7.2, 1.8 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 2H), 7.18 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 6.42 (s, 1H), 3.96 (s, 3H), 3.72 (s, 3H), 3.23 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 157.4, 156.3, 156.1, 144.9, 135.5, 135.0, 130.9, 129.8, 126.9, 126.3, 124.5, 123.2, 121.5, 115.0, 113.7, 109.0, 92.9, 60.5, 56.5, 56.1, 21.6; HRMS (ESI) *m/z*: 494.0805, 496.0774 (Calcd for $C_{24}H_{22}ClNO_5SNa$ $[M+Na]^+$: 494.0805, 496.0775).

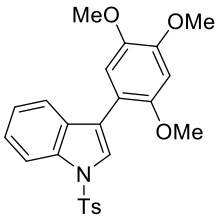
1-Tosyl-3-(2,4,6-trimethoxy-[1,1'-biphenyl]-3-yl)indole (5ad)



5ad

0.3 mmol scale: 117 mg, 76% yield. colorless solid; mp 174–175 °C; IR (KBr): 1456, 1383, 1172, 1109 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 8.4 Hz, 1H), 7.77 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.66 (s, 1H), 7.40–7.39 (m, 4H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.33–7.27 (m, 2H), 7.19 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 2H), 6.46 (s, 1H), 3.80 (s, 3H), 3.76 (s, 3H), 2.84 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 158.4, 158.1, 157.9, 144.7, 135.6, 135.0, 134.2, 131.3, 131.0, 129.8, 127.9, 126.9, 126.8, 126.1, 124.3, 123.1, 121.7, 117.8, 116.0, 113.6, 107.7, 92.0, 60.4, 56.1, 55.9, 21.6; HRMS (ESI) *m/z*: 536.1508 (Calcd for $C_{30}H_{27}NO_5SNa$ $[M+Na]^+$: 536.1508).

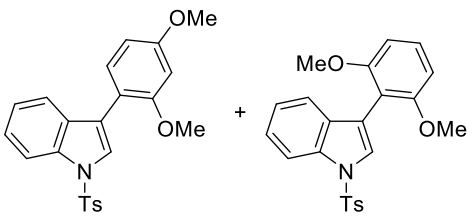
1-Tosyl-3-(2,4,5-trimethoxyphenyl)indole (5ae)



5ae

270 mg, 62% yield. colorless solid; mp 133–135 °C; IR (KBr): 1447, 1364, 1211, 1169, 1125 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 8.4 Hz, 1H), 7.80 (ddd, *J* = 7.8, 1.8, 1.8 Hz, 2H), 7.75 (s, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.32 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 7.25–7.21 (m, 3H), 7.02 (s, 1H), 6.65 (s, 1H), 3.95 (s, 3H), 3.86 (s, 3H), 3.76 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 151.5, 149.3, 144.9, 143.2, 135.4, 135.1, 130.4, 129.9, 127.0, 125.0, 124.5, 123.3, 121.0, 119.4, 114.4, 113.8, 113.3, 98.4, 56.8, 56.6, 56.3, 21.7; HRMS (ESI) *m/z*: 460.1195 (Calcd for $C_{24}H_{23}NO_5SNa$ $[M+Na]^+$: 460.1195).

Mixture of 3-(2,4-dimethoxyphenyl)-1-tosylindole (5af) and 3-(2,6-dimethoxyphenyl)-1-tosylindole (5af')

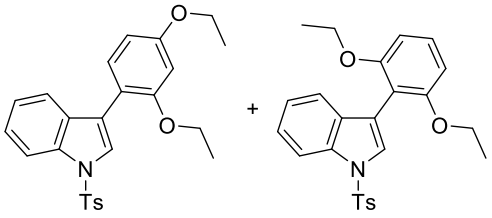


5af **5af'** mixture of regioisomers

249 mg, 61% yield. colorless oil; IR (KBr): 1447, 1369, 1175, 1128 cm^{-1}; **5af**: ^1H NMR (600 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 7.8 Hz, 2H), 7.72 (s, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.30 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.23–7.20 (m, 3H), 6.59 (d, *J* = 2.4 Hz, 1H), 6.57 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.85 (s,

3H), 3.80 (s, 3H), 2.32 (s, 3H); **5af'**: ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.98 (d, *J* = 7.2 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.65 (s, 1H), 7.32–7.20 (m, 5H), 7.15 (ddd, *J* = 8.4, 7.8, 0.6 Hz, 1H), 6.66 (d, *J* = 8.4 Hz, 2H), 3.71 (s, 6H), 2.32 (s, 3H); mixture of **5af** and **5af'**: ^{13}C NMR (151 MHz, $CDCl_3$) δ: 160.5, 158.5, 158.1, 144.8, 144.7, 135.6, 135.5, 135.1, 134.9, 131.3, 131.2, 130.6, 129.9, 129.8, 129.4, 127.2, 127.0, 126.7, 124.8, 124.4, 124.0, 123.2, 122.9, 121.7, 121.2, 119.5, 115.2, 114.5, 113.7, 113.5, 110.1, 104.5, 104.2, 99.2, 55.9, 55.6, 55.6, 21.6, 21.6; HRMS (ESI) *m/z*: 430.1090 (Calcd for $C_{23}H_{21}NO_4SNa$ $[M+Na]^+$: 430.1089).

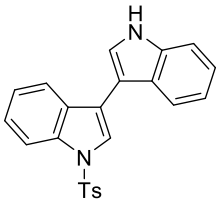
Mixture of 3-(2,4-diethoxyphenyl)-1-tosylindole (5ag) and 3-(2,6-diethoxyphenyl)-1-tosylindole (5ag')



5ag **5ag'** mixture of regioisomers

230 mg, 53% yield. colorless oil; IR (KBr): 1447, 1369, 1175, 1132 cm^{-1}; **5ag**: ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.05 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 2H), 7.79 (s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 6.6 Hz, 1H), 7.26–7.14 (m, 3H), 6.58 (d, *J* = 2.4 Hz, 1H), 6.56 (dd, *J* = 8.4, 2.4 Hz, 1H), 4.08 (q, *J* = 6.6 Hz, 2H), 4.03 (q, *J* = 6.6 Hz, 2H), 2.31 (s, 3H), 1.44 (t, *J* = 7.2 Hz, 3H), 1.36 (t, *J* = 7.2 Hz, 3H); **5ag'**: ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.00 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 2H), 7.68 (s, 1H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.26–7.14 (m, 5H), 6.63 (d, *J* = 7.8 Hz, 2H), 3.95 (q, *J* = 6.6 Hz, 4H), 2.31 (s, 3H), 1.17 (t, *J* = 7.2 Hz, 6H); mixture of **5ag** and **5ag'**: ^{13}C NMR (151 MHz, $CDCl_3$) δ: 159.7, 157.8, 157.3, 144.8, 144.6, 135.7, 135.5, 135.1, 134.8, 131.2, 130.9, 130.6, 129.9, 129.8, 129.2, 126.9, 126.9, 126.6, 125.0, 124.4, 123.9, 123.1, 122.5, 122.2, 121.1, 119.3, 115.5, 114.4, 113.7, 113.3, 110.5, 105.2, 105.1, 100.5, 64.1, 63.9, 63.7, 21.6, 21.6, 15.0, 14.9, 14.8; HRMS (ESI) *m/z*: 458.1403 (Calcd for $C_{25}H_{25}NO_4SNa$ $[M+Na]^+$: 458.1402).

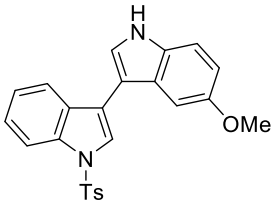
3-(Indol-3-yl)-1-tosylindole (5ah)



5ah

287 mg, 74% yield. colorless oil; IR (KBr): 3422, 1447, 1364, 1173 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.31 (br s, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.82–7.80 (m, 3H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 2.4 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.36 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.29–7.25 (m, 2H), 7.21–7.20 (m, 3H), 2.31 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.9, 136.4, 135.5, 135.3, 130.5, 130.0, 126.9, 126.3, 124.9, 123.4, 122.9, 122.6, 122.5, 120.9, 120.5, 120.0, 117.4, 114.0, 111.5, 108.9, 21.6; HRMS (ESI) *m/z*: 409.0987 (Calcd for $C_{23}H_{18}N_2O_2SNa$ $[M+Na]^+$: 409.0987).

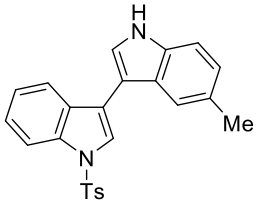
3-(5-Methoxyindol-3-yl)-1-tosylindole (5ai)



5ai

250 mg, 60% yield. colorless oil; IR (KBr): 3422, 1447, 1364, 1173 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.24 (br s, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 7.81 (ddd, *J* = 9.0, 1.8, 1.8 Hz, 2H), 7.76 (s, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.36 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.33 (d, *J* = 9.0 Hz, 1H), 7.26 (ddd, *J* = 8.4, 6.6, 1.8 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.18 (d, *J* = 2.4 Hz, 1H), 6.93 (dd, *J* = 9.0, 3.0 Hz, 1H), 3.84 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 154.8, 145.0, 135.5, 135.4, 131.5, 130.5, 130.0, 126.9, 126.9, 124.9, 123.4, 122.4, 120.9, 117.5, 114.0, 113.0, 112.2, 108.6, 101.9, 56.1, 21.6; HRMS (ESI) *m/z*: 439.1093 (Calcd for $C_{24}H_{20}N_2O_3SNa$ $[M+Na]^+$: 439.1092).

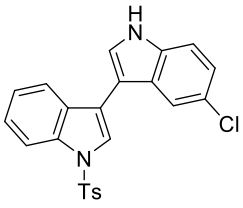
3-(5-Methylindol-3-yl)-1-tosylindole (5aj)



5aj

323 mg, 81% yield. colorless oil; IR (KBr): 3420, 1447, 1364, 1175 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.23 (br s, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.82–7.81 (m, 3H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.57 (s, 1H), 7.40–7.39 (m, 2H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.27 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.10 (dd, *J* = 8.4, 1.2 Hz, 1H), 3.67 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.0, 135.5, 135.3, 134.7, 130.6, 130.0, 129.8, 126.9, 126.5, 124.9, 124.5, 123.5, 122.8, 122.4, 121.0, 119.5, 117.7, 114.0, 111.2, 108.2, 21.7, 21.6; HRMS (ESI) *m/z*: 423.1143 (Calcd for $C_{24}H_{20}N_2O_2SNa$ $[M+Na]^+$: 423.1143).

3-(5-Chloroindol-3-yl)-1-tosylindole (5ak)

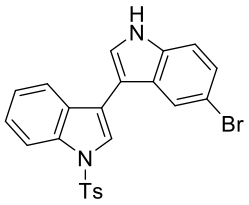


5ak

270 mg, 64% yield. colorless solid; mp 149–150 °C; IR (KBr): 3435, 1449, 1368, 1169, 1086 cm^{-1}; ^1H NMR (600

MHz, $CDCl_3$) δ: 8.40 (br s, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.82 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.75 (s, 1H), 7.68 (d, *J* = 1.8 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 3.0 Hz, 1H), 7.37 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.33 (d, *J* = 9.0 Hz, 1H), 7.27 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.21–7.20 (m, 3H), 2.31 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.1, 135.5, 135.2, 134.7, 130.3, 130.0, 127.5, 126.9, 126.2, 125.1, 124.0, 123.6, 123.2, 122.6, 120.7, 119.4, 116.8, 114.0, 112.6, 108.6, 21.7; HRMS (ESI) *m/z*: 443.0596, 445.0568 (Calcd for $C_{23}H_{17}ClN_2O_2SNa$ $[M+Na]^+$: 443.0597, 445.0568).

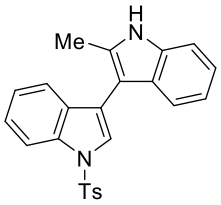
3-(5-Bromoindol-3-yl)-1-tosylindole (5al)



5al

256 mg, 55% yield. colorless solid; mp 154–156 °C; IR (KBr): 3433, 1447, 1368, 1171, 1094 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.38 (br s, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.83–7.81 (m, 3H), 7.73 (s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 2.4 Hz, 1H), 7.37 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.34 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.27 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.1, 135.5, 135.2, 135.0, 130.3, 130.0, 128.2, 126.9, 125.7, 125.1, 123.8, 123.6, 122.7, 122.5, 120.7, 116.8, 114.0, 113.7, 113.0, 108.5, 21.7; HRMS (ESI) *m/z*: 487.0091, 489.0070 (Calcd for $C_{23}H_{17}BrN_2O_2SNa$ $[M+Na]^+$: 487.0092, 489.0071).

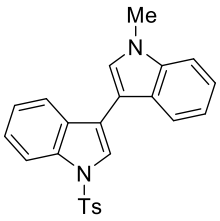
3-(2-Methylindol-3-yl)-1-tosylindole (5am)



5am

287 mg, 71% yield. colorless solid; mp 103–105 °C; IR (KBr): 3399, 1458, 1364, 1173 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.10 (br s, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.83 (ddd, *J* = 9.0, 1.8, 1.8 Hz, 2H), 7.58 (s, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.36 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.34 (d, *J* = 8.4 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.22 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 7.17 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.07 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 2.42 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.0, 135.5, 135.4, 135.3, 132.9, 131.3, 130.0, 128.4, 127.0, 124.8, 124.0, 123.2, 121.7, 121.6, 119.9, 119.3, 117.3, 113.9, 110.5, 105.0, 21.7, 12.7; HRMS (ESI) *m/z*: 423.1142 (Calcd for $C_{24}H_{20}N_2O_2SNa$ $[M+Na]^+$: 423.1143).

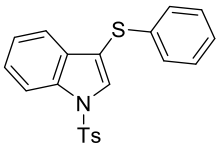
3-(1-Methylindol-3-yl)-1-tosylindole (5an)



5an

208 mg, 52% yield. red oil; IR (KBr): 1447, 1368, 1175 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.09 (d, *J* = 8.4 Hz, 1H), 7.82 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.80–7.79 (m, 2H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.37 (ddd, *J* = 8.4, 6.6, 1.8 Hz, 1H), 7.34 (s, 1H), 7.32 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 7.27 (ddd, *J* = 8.4, 7.8, 0.6 Hz, 1H), 7.21 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 2H), 3.86 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 144.9, 137.2, 135.5, 135.4, 130.5, 129.9, 127.2, 126.9, 126.8, 124.9, 123.4, 122.4, 122.2, 120.9, 120.2, 120.0, 117.6, 114.0, 109.7, 107.2, 33.1, 21.6; HRMS (ESI) *m/z*: 423.1144 (Calcd for $C_{24}H_{20}N_2O_2SNa$ $[M+Na]^+$: 423.1143).

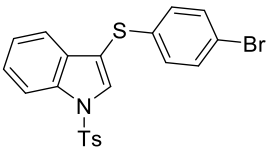
3-Phenylthio-1-tosylindole (5ao)



5ao

190 mg, 50% yield. colorless oil; IR (KBr): 1445, 1373, 1265, 1175 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.00 (d, *J* = 8.4 Hz, 1H), 7.82 (s, 1H), 7.79 (ddd, *J* = 9.0, 1.8, 1.8 Hz, 2H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.34 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.20 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 7.18–7.15 (m, 2H), 7.12–7.08 (m, 3H), 2.36 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.5, 136.3, 135.5, 135.0, 131.1, 130.9, 130.1, 129.0, 127.3, 127.1, 125.9, 125.5, 123.9, 120.5, 113.9, 111.9, 21.7; HRMS (ESI) *m/z*: 402.0598 (Calcd for $C_{21}H_{17}NO_2S_2Na$ $[M+Na]^+$: 402.0598).

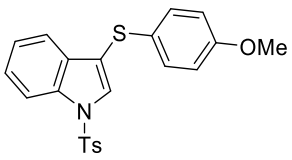
3-(4-Bromophenylthio)-1-tosylindole (5ap)



5ap

321 mg, 70% yield. colorless solid; mp 149–151 °C; IR (KBr): 1474, 1369, 1260, 1167, 1005 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.00 (d, *J* = 8.4 Hz, 1H), 7.83 (s, 1H), 7.80 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.35 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.28–7.25 (m, 4H), 7.21 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.20 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 6.93 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.6, 135.7, 135.5, 134.9, 132.0, 131.2, 130.8, 130.2, 128.7, 127.1, 125.7, 124.0, 120.4, 119.6, 113.9, 111.0, 21.7; HRMS (ESI) *m/z*: 479.9704, 481.9682 (Calcd for $C_{21}H_{16}BrNO_2S_2Na$ $[M+Na]^+$: 479.9704, 481.9683).

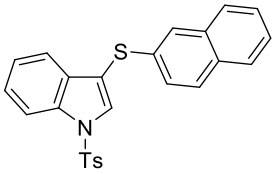
3-(4-Methoxyphenylthio)-1-tosylindole (5aq)



5aq

82.6 mg, 20% yield. colorless oil; IR (KBr): 1493, 1373, 1265, 1175 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 8.4 Hz, 1H), 7.81 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.75 (s, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.36 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.26–7.21 (m, 5H), 6.80 (ddd, *J* = 9.6, 2.4, 2.4 Hz, 2H), 3.78 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 158.8, 145.4, 135.5, 135.0, 131.0, 130.9, 130.1, 129.3, 127.0, 125.9, 125.4, 123.8, 120.4, 114.8, 114.4, 113.8, 55.4, 21.7; HRMS (ESI) *m/z*: 432.0704 (Calcd for $C_{22}H_{19}NO_3S_2Na$ $[M+Na]^+$: 432.0704).

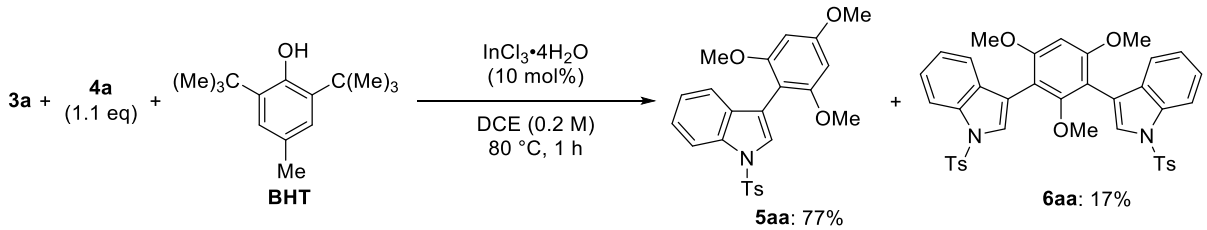
3-(2-Naphthalenylthio)-1-tosylindole (5ar)



5ar

228 mg, 53% yield. colorless oil; IR (KBr): 1445, 1375, 1263, 1175 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 9.0 Hz, 1H), 7.87 (s, 1H), 7.81 (ddd, *J* = 9.0, 1.8, 1.8 Hz, 2H), 7.73 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.53 (d, *J* = 9.0 Hz, 1H), 7.48 (d, *J* = 1.8 Hz, 1H), 7.42–7.37 (m, 3H), 7.34 (ddd, *J* = 8.4, 0.6, 0.6 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.22 (dd, *J* = 9.0, 1.8 Hz, 1H), 7.17 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.5, 135.5, 135.0, 133.7, 133.7, 131.8, 131.1, 131.0, 130.2, 128.7, 127.8, 127.1, 127.1, 126.6, 125.7, 125.6, 125.4, 124.0, 120.5, 113.9, 111.9, 21.7; HRMS (ESI) *m/z*: 452.0755 (Calcd for $C_{25}H_{19}NO_2S_2Na$ $[M+Na]^+$: 452.0755).

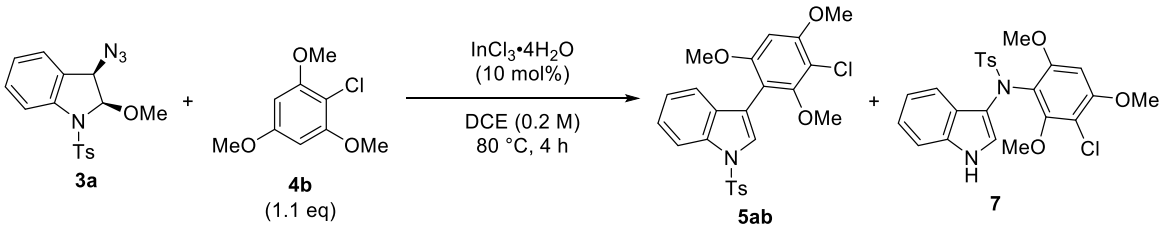
■Control experiment: reaction of 3 with 2,6-di-*tert*-butyl-4-hydroxytoluene (BHT) as radical scavenger



To a solution of **3a** (104 mg, 0.3 mmol), **4a** (56.0 mg, 0.33 mmol) and BHT (68.3 mg, 0.3 mmol) in DCE (1.5 mL, 0.2 M) was added $InCl_3$•$4H_2O$ (8.8 mg, 0.03 mmol) under Ar. The mixture was allowed to stir at 80 °C for 1 h in oil bath. After H_2O (0.1 mL) was added to the mixture at 80 °C, and the mixture was stirred at 80 °C for 30 min. The reaction mixture was cooled to room temperature and diluted with H_2O (10 mL). Then, the whole was extracted with $CHCl_3$ (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/10–1/2) to give **5aa** (101 mg,

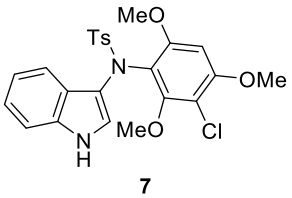
77%) and **6aa** (18.2 mg, 17%).

■Isolation of the intermediate 7



To a solution of **3a** (345 mg, 1 mmol) and 1-chloro-2,4,6-trimethoxybenzene **4b** (224 mg, 1.1 mmol) in DCE (5 mL, 0.2 M) was added $InCl_3$•$4H_2O$ (29.5 mg, 0.1 mmol) under Ar. The mixture was allowed to stir for 4 h at 80 °C in oil bath. After H_2O (1 mL) was added to the mixture at 80 °C, and the mixture was stirred at 80 °C for 30 min. The reaction mixture was cooled to room temperature and diluted with H_2O (10 mL). Then, extracted with $CHCl_3$ (3 x 25 mL), washed with brine (25 mL). The combined organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/10–1/1) to give **5ac** (324 mg, 69%) and **7** (9.2 mg, 2%). This structure of **7** was determined by 2D NMR (H-H COSY, HMQC, HMBC).

3-[*N*-(3-chloro-2,4,6-trimethoxyphenyl)-*N*-tosylamino]indole (7)

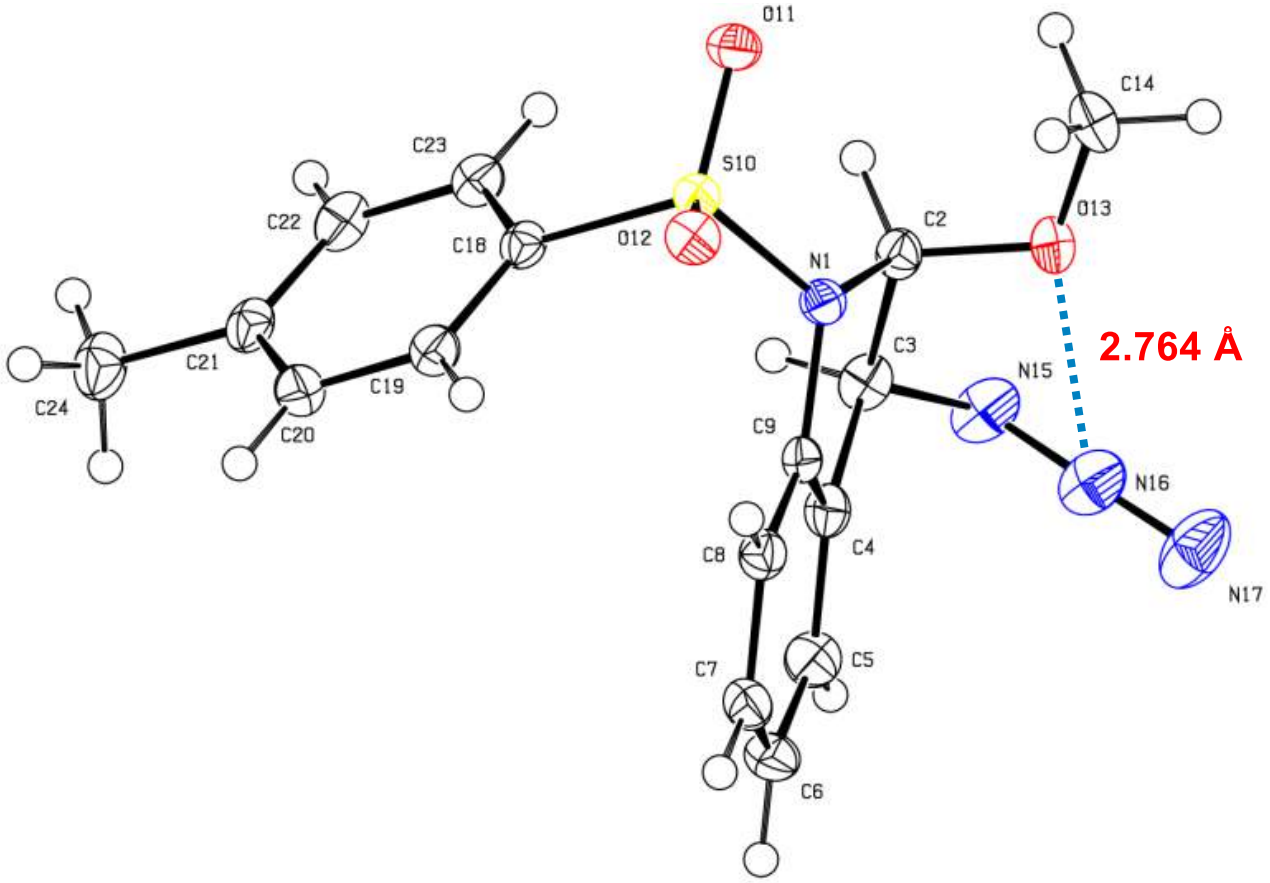


9.2 mg, 2% yield. orange oil; IR (KBr): 3379, 1456, 1341, 1161, 1107 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ: 8.35 (br s, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.26 (ddd, *J* = 8.4, 1.8, 1.8 Hz, 2H), 7.22 (ddd, *J* = 7.8, 6.6, 1.2 Hz, 1H), 7.19 (ddd, *J* = 7.8, 6.6, 1.2 Hz, 1H), 7.13 (s, 1H), 6.80 (d, *J* = 8.4 Hz, 2H), 6.20 (s, 1H), 3.95 (s, 3H), 3.71 (s, 3H), 3.25 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 156.7, 155.7, 154.4, 142.0, 136.4, 134.8, 128.6, 127.1, 126.1, 125.0, 123.1, 120.5, 119.9, 111.7, 110.7, 109.8, 107.4, 92.8, 61.1, 56.6, 56.4, 21.6; HRMS (ESI) *m/z*: 509.0912, 511.0884 (Calcd for $C_{24}H_{23}ClN_2O_5SNa$ $[M+Na]^+$: 509.0914, 511.0884).

3. X-ray crystallographic Analysis

The structure of **3a** was also elucidated by X-ray crystallographic analysis. The single crystal for the analysis was grown by vapor diffusion of hexane to $CHCl_3$ solution of **3a**. The data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. CCDC 2107262 contains the supplementary crystallographic data for this paper.

Figure S1 ORTEP drawing of 3a and indication of O–N bonding



ORTEP drawing of **3a**

The dashed line in the figure indicates O–N bonding. Nitrogen is depicted in blue, oxygen in red, sulfur in yellow, carbon in black. The interatomic distances between N2 of azide (labeled as N16) and the closest oxygen atom (labeled as O13) are given in figure S1.

X-ray structure, crystal data and thermal ellipsoid plots of **3a** (at the 50% probability level unless otherwise stated).

Table S3 Crystal data of 3a

Empirical formula	$C_{16}H_{16}N_4O_3S$
Formula weight	334.39
Crystal system	Orthorhombic
Space group [No.]	*P b c a* [61]
Crystal color, habit	Colorless, block
Crystal size	0.90×0.29×0.11 mm
Unit cell parameters	a = 18.1042(1) Å b = 8.5594(1) Å c = 21.0097(1) Å α = 90º β = 90º γ = 90º
Temperature	103 K
Wavelength	1.54184 Å
Volume	3255.69(4) $Å^3$
Z	8
F(000)	1440.0
h, *k*, *l*, max	21, 8, 25
R1 (*I* > 2.00σ(i))	0.0287
R (all reflection)	0.0294
GOF	1.049

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S4 Bond distance in angstroms of 3a

atom 1	atom 2	distance	atom 1	atom 2	distance
S10	N1	1.649(1)	C4	C5	1.381(2)
S10	O11	1.4349(9)	C4	C9	1.389(2)
S10	O12	1.431(1)	C5	C6	1.392(2)
S10	C18	1.759(1)	C6	C7	1.386(2)
O13	C2	1.393(2)	C7	C8	1.394(2)
O13	C14	1.433(2)	C8	C9	1.386(2)
N1	C2	1.493(2)	C18	C19	1.393(2)
N1	C9	1.435(2)	C18	C23	1.392(2)
N15	N16	1.246(2)	C19	C20	1.384(2)
N15	C3	1.478(2)	C20	C21	1.395(2)
N16	N17	1.132(2)	C21	C22	1.393(2)
C2	C3	1.549(2)	C21	C24	1.505(2)
C3	C4	1.509(2)	C22	C23	1.384(2)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S5 Bond angle in degrees of 3a

atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle
O11	S10	N1	105.48(5)	C3	C4	C9	109.8(1)
O11	S10	O12	119.81(6)	C5	C4	C9	120.6(1)
O11	S10	C18	109.67(6)	C4	C5	C6	118.6(1)
O12	S10	N1	107.29(6)	C5	C6	C7	120.3(1)
O12	S10	C18	107.39(6)	C6	C7	C8	121.7(1)
N1	S10	C18	106.45(6)	C7	C8	C9	117.0(1)
C2	O13	C14	112.6(1)	N1	C9	C4	109.9(1)
S10	N1	C2	121.38(8)	N1	C9	C8	128.2(1)
S10	N1	C9	119.92(9)	C4	C9	C8	121.8(1)
C2	N1	C9	108.4(1)	S10	C18	C19	119.3(1)
N16	N15	C3	113.5(1)	S10	C18	C23	119.8(1)
N15	N16	N17	172.4(2)	C19	C18	C23	120.8(1)
O13	C2	N1	110.2(1)	C18	C19	C20	119.1(1)
O13	C2	C3	108.9(1)	C19	C20	C21	121.2(1)
N1	C2	C3	103.6(1)	C20	C21	C22	118.4(1)
N15	C3	C2	114.5(1)	C20	C21	C24	120.2(1)
N15	C3	C4	115.6(1)	C22	C21	C24	121.3(1)
C2	C3	C4	103.5(1)	C21	C22	C23	121.4(1)
C3	C4	C5	129.6(1)	C18	C23	C22	119.0(1)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S6 Torsion angles in degrees of 3a

atom 1	atom 2	atom 3	atom 4	angle
O11	S10	N1	C2	-27.2(1)
O11	S10	N1	C9	-168.11(9)
O12	S10	N1	C2	-155.97(9)
O12	S10	N1	C9	63.1(1)
C18	S10	N1	C2	89.3(1)
C18	S10	N1	C9	-51.6(1)
O11	S10	C18	C19	-152.2(1)
O11	S10	C18	C23	29.5(1)
O12	S10	C18	C19	-20.5(1)
O12	S10	C18	C23	161.2(1)
N1	S10	C18	C19	94.2(1)
N1	S10	C18	C23	-84.1(1)
C14	O13	C2	N1	-71.3(1)
C14	O13	C2	C3	175.7(1)
S10	N1	C2	O13	119.9(1)
S10	N1	C2	C3	-123.7(1)
C9	N1	C2	O13	-95.2(1)
C9	N1	C2	C3	21.2(1)
S10	N1	C9	C4	132.1(1)
S10	N1	C9	C8	-47.7(2)
C2	N1	C9	C4	-13.3(1)
C2	N1	C9	C8	166.9(1)
N16	N15	C3	C2	78.9(1)
N16	N15	C3	C4	-41.3(2)
C3	N15	N16	N17	171(1)
O13	C2	C3	N15	-30.1(1)
O13	C2	C3	C4	96.6(1)

atom 1	atom 2	atom 3	atom 4	angle
N1	C2	C3	N15	-147.4(1)
N1	C2	C3	C4	-20.7(1)
N15	C3	C4	C5	-41.6(2)
N15	C3	C4	C9	139.9(1)
C2	C3	C4	C5	-167.7(1)
C2	C3	C4	C9	13.8(1)
C3	C4	C5	C6	-178.1(1)
C9	C4	C5	C6	0.2(2)
C3	C4	C9	N1	-0.8(1)
C3	C4	C9	C8	179.0(1)
C5	C4	C9	N1	-179.5(1)
C5	C4	C9	C8	0.3(2)
C4	C5	C6	C7	-0.4(2)
C5	C6	C7	C8	0.0(2)
C6	C7	C8	C9	0.5(2)
C7	C8	C9	N1	179.1(1)
C7	C8	C9	C4	-0.6(2)
S10	C18	C19	C20	-178.7(1)
C23	C18	C19	C20	-0.4(2)
S10	C18	C23	C22	179.2(1)
C19	C18	C23	C22	0.9(2)
C18	C19	C20	C21	-1.0(2)
C19	C20	C21	C22	1.8(2)
C19	C20	C21	C24	-177.7(1)
C20	C21	C22	C23	-1.3(2)
C24	C21	C22	C23	178.2(1)
C21	C22	C23	C18	-0.1(2)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S7 Atomic coordinates for 3a

atom	Xfrac + ESD	Yfrac + ESD	Zfrac + ESD	atom	Xfrac + ESD	Yfrac + ESD	Zfrac + ESD
S10	0.37962(2)	0.50891(3)	0.41332(2)	C21	0.25745(7)	0.25218(15)	0.57062(6)
O11	0.33091(5)	0.61732(10)	0.38247(4)	C22	0.21984(7)	0.30742(16)	0.51731(6)
O12	0.44807(5)	0.56268(11)	0.43936(4)	C23	0.25623(7)	0.38641(15)	0.46917(6)
O13	0.38095(5)	0.36995(12)	0.24750(4)	C24	0.21742(8)	0.17045(18)	0.62384(7)
N1	0.39947(6)	0.37621(12)	0.35903(5)	H2	0.300215	0.400206	0.310459
N15	0.32149(6)	0.08024(15)	0.25151(6)	H3	0.289005	0.147356	0.339299
N16	0.37939(7)	0.05352(16)	0.22135(6)	H5	0.399701	-0.130523	0.343578
N17	0.42728(8)	0.0196(2)	0.18962(7)	H6	0.503388	-0.166578	0.409247
C2	0.34736(7)	0.34035(16)	0.30594(6)	H7	0.563367	0.047355	0.45334
C3	0.33407(7)	0.16228(16)	0.31245(6)	H8	0.522288	0.303637	0.433464
C4	0.39963(7)	0.10689(15)	0.35059(6)	H14A	0.410884	0.548609	0.192848
C5	0.42424(8)	-0.04332(16)	0.36189(7)	H14B	0.424108	0.577923	0.267209
C6	0.48577(8)	-0.06416(17)	0.40071(7)	H14C	0.342348	0.586195	0.238452
C7	0.52147(8)	0.06384(17)	0.42696(6)	H19	0.422915	0.37181	0.529965
C8	0.49747(7)	0.21614(16)	0.41567(6)	H20	0.360229	0.235869	0.609555
C9	0.43576(7)	0.23410(15)	0.37729(6)	H22	0.168127	0.290495	0.513959
C14	0.39031(9)	0.53361(19)	0.23556(7)	H23	0.229897	0.423338	0.433065
C18	0.33199(7)	0.41096(14)	0.47442(6)	H24A	0.164067	0.185251	0.618732
C19	0.37116(7)	0.35527(15)	0.52677(6)	H24B	0.233173	0.21426	0.664735
C20	0.33363(7)	0.27549(16)	0.57408(6)	H24C	0.228936	0.058613	0.622691

Numbers in parentheses are estimated standard deviations in the least significant digits.

4. Supplementary References

[S1] Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3–8.

[S2] Sheldrick, G. M. *Acta Cryst.* **2015**, *C71*, 3–8.

[S3] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339–341.

[S4] ***N*-tosylation, *N*-benzenesulfonylation, and *N*-2-nosylation:** Hodson, H. F.; Madge, D. J.; Slawin, A. N. Z.; Widdowson, D. A.; Williams, D. J. *Tetrahedron* **1994**, *50*, 1899–1906.

[S5] ***N*-benzoylation:** Lanke, V.; Prebhu, K. R. *Org., Lett.* **2013**, *15*, 2818–2821.

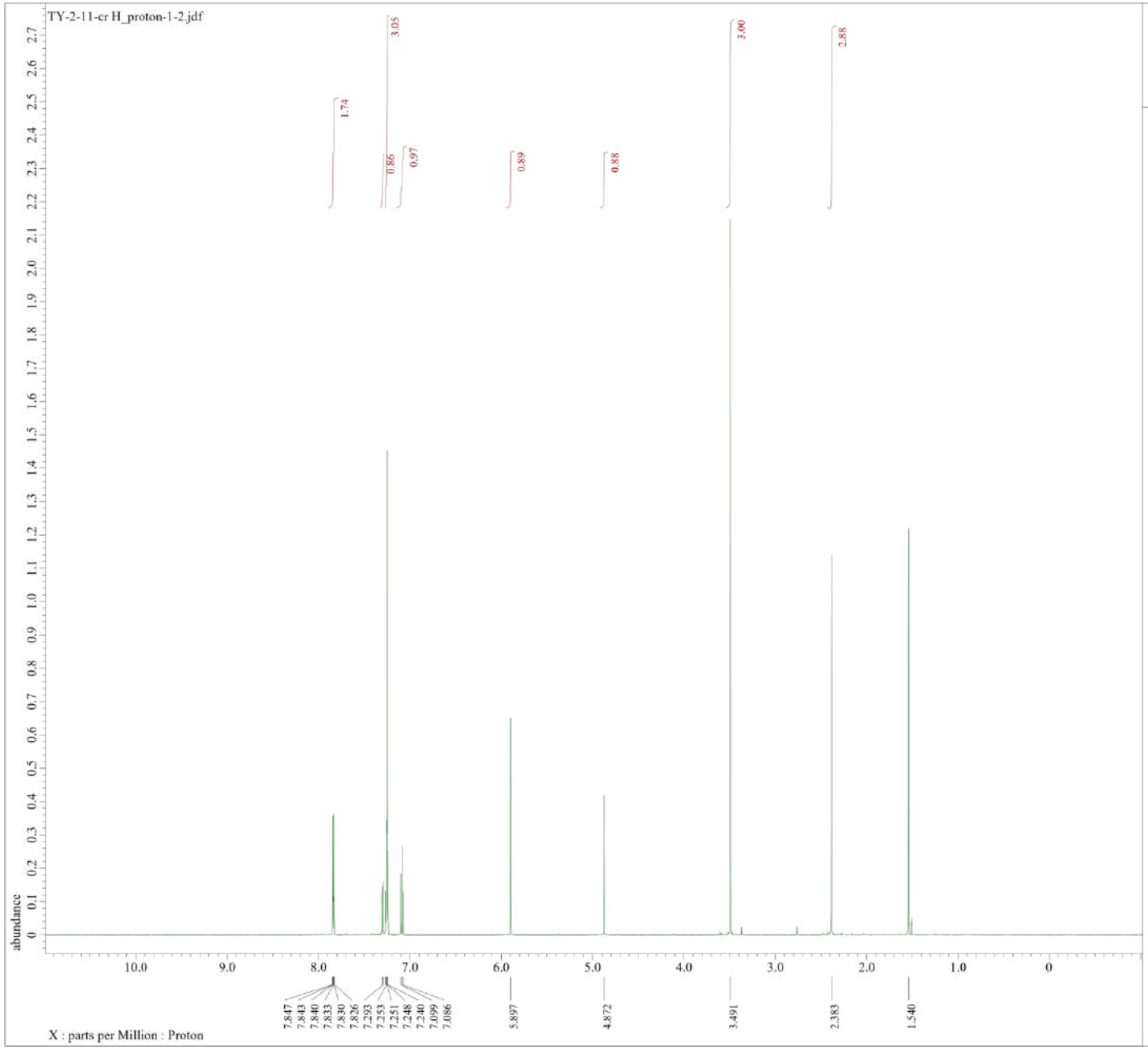
[S6] ***N*-acetylation:** Medina-Mercado, I.; Asomoza-Solís, E. O.; Martínez-González, E.; Ugalde-Saldívar, V. M.; Ledesma-Olvera, L. G.; Barquera-Lozada, J. E.; Gómez-Vidales, V.; Barroso-Flores, J.; Frontana-Uribe, B. A.; Porcel, S. *Chem. Eur. J.* **2020**, *26*, 634–642.

[S7] Synthesis of 3-bromo-2-alkoxy-indolines: Abe, T.; Kosaka, Y.; Kawasaki, T.; Ohata, Y.; Yamashiro, T.; Yamada, K. *Chem. Pharm. Bull.* **2020**, *68*, 555–558.

[S8] Synthesis of 1-bromo-2,4,6-trimethoxybenzene: Mondal, M.; Puranik, V. G.; Argade, N. P. *J. Org. Chem.* **2006**, *71*, 4992–4995.

[S9] Synthesis of 1-chloro-2,4,6-trimethoxybenzene: Tang, R.-J.; Milcent, T.; Crousse, B. *J. Org. Chem.* **2018**, *83*, 930–938.

[S10] Synthesis of 1-phenyl-2,4,6-trimethoxybenzene: Wang, X.; Huang, D.; Wang, X.; Zeng, X.; Wang, X.; Huhn, Y. *Tetrahedron Lett.* **2016**, *57*, 4235–4238.



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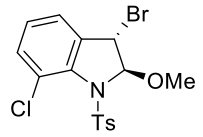

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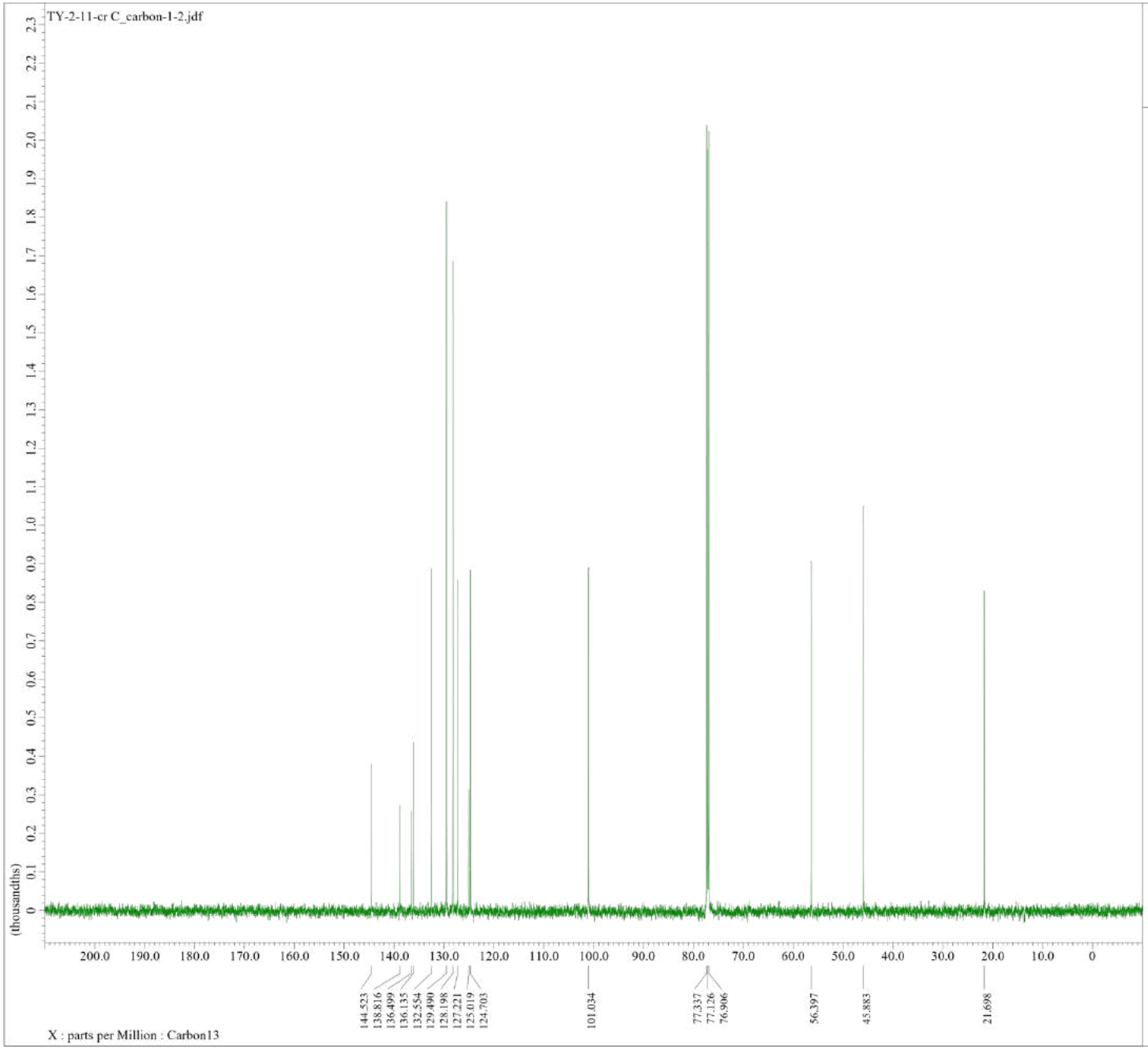

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X_Sweep_Clipped	= 37.87878788[kHz]
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Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
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Total_Scans	= 256
Relaxation_Delay	= 2[s]
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Temp_Get	= 20.8[dC]
X_90_Width	= 11.8[us]
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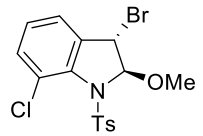

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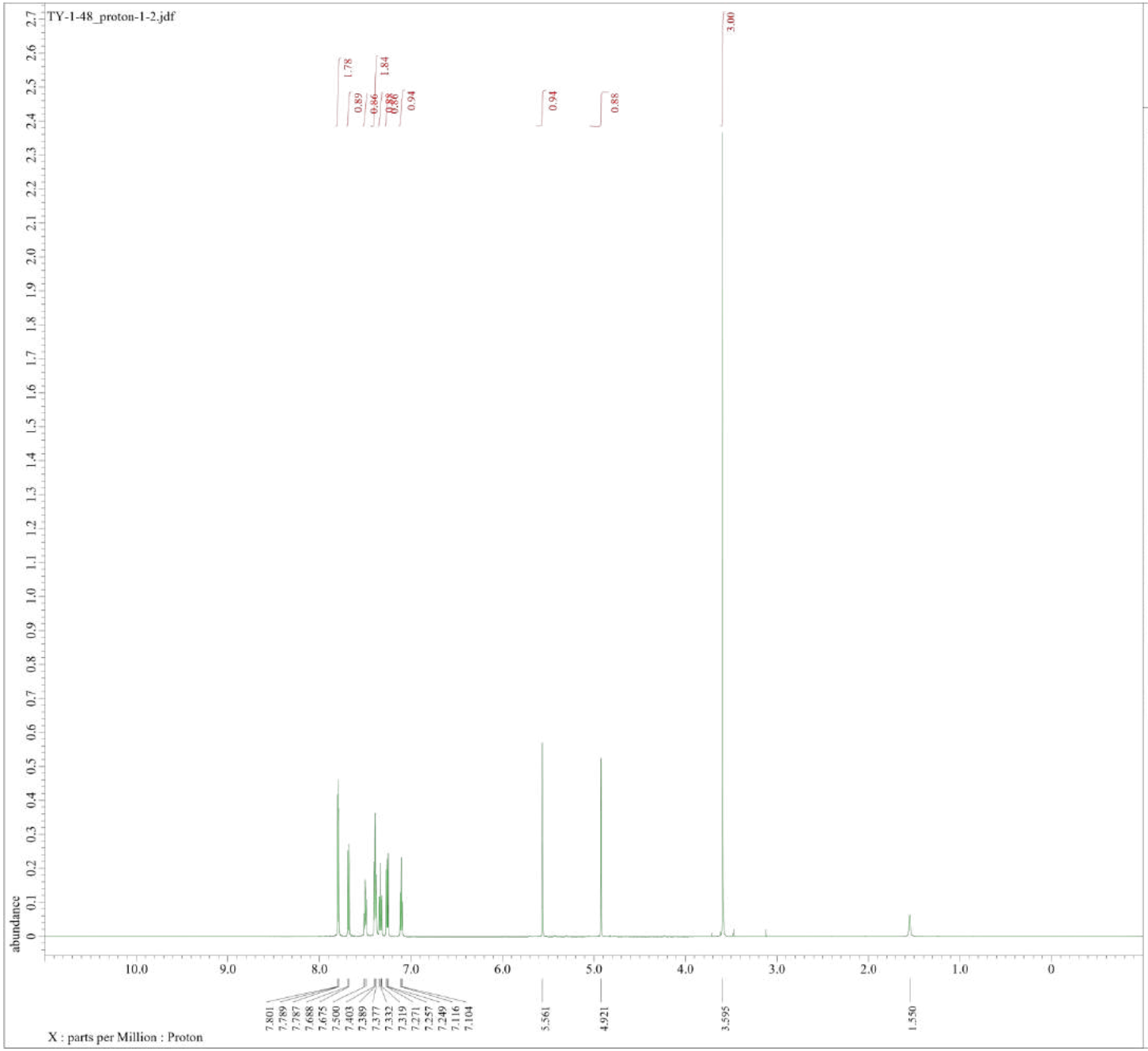

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X_Sweep_Clipped	= 12.01923077[kHz]
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Clipped	= FALSE
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Temp_Get	= 20.5[dC]
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X_Atn	= 8.1[dB]
X_Pulse	= 4.75[us]
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Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
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Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
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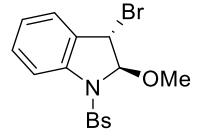

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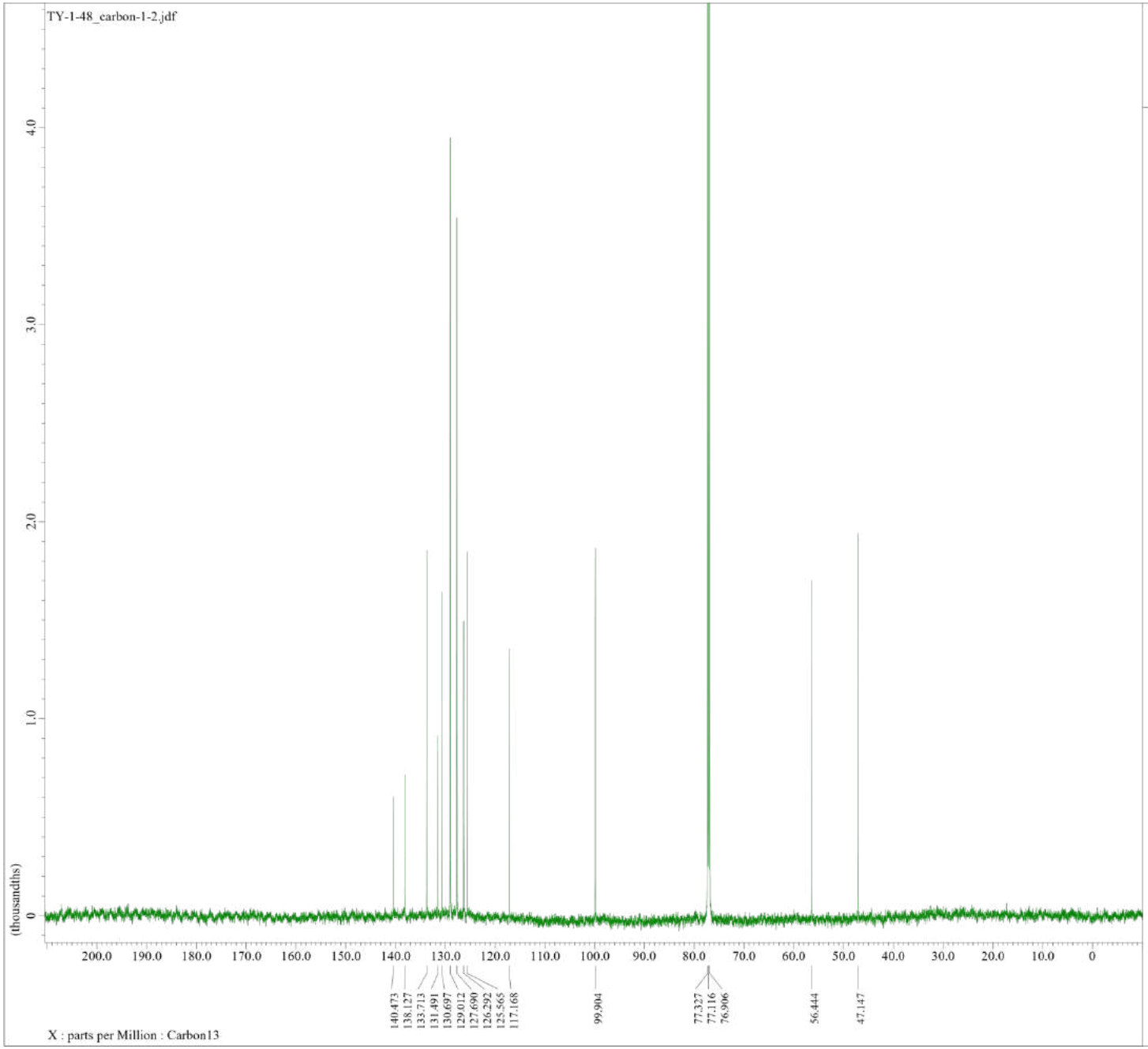

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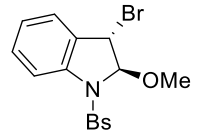

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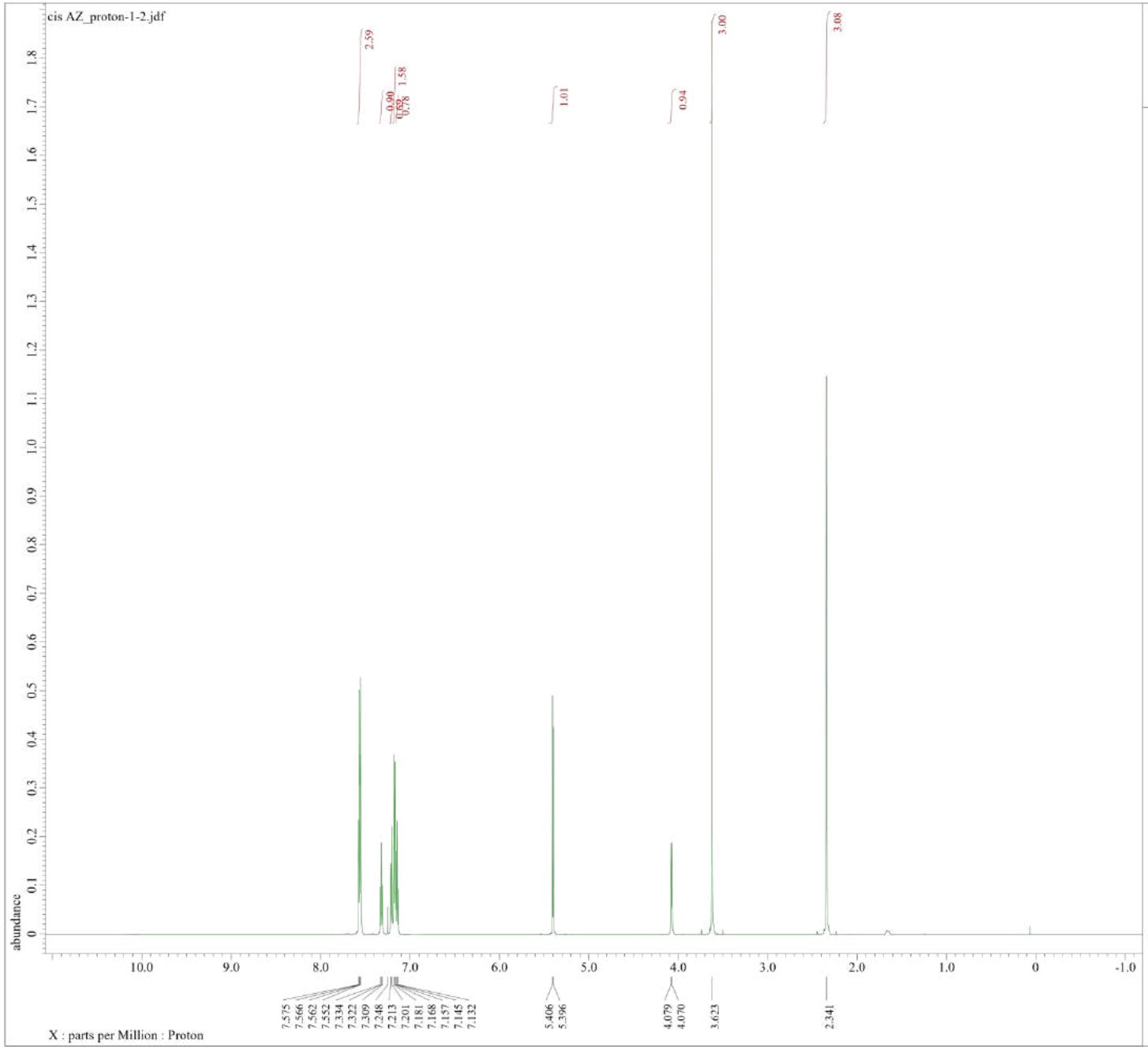

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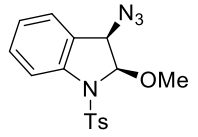
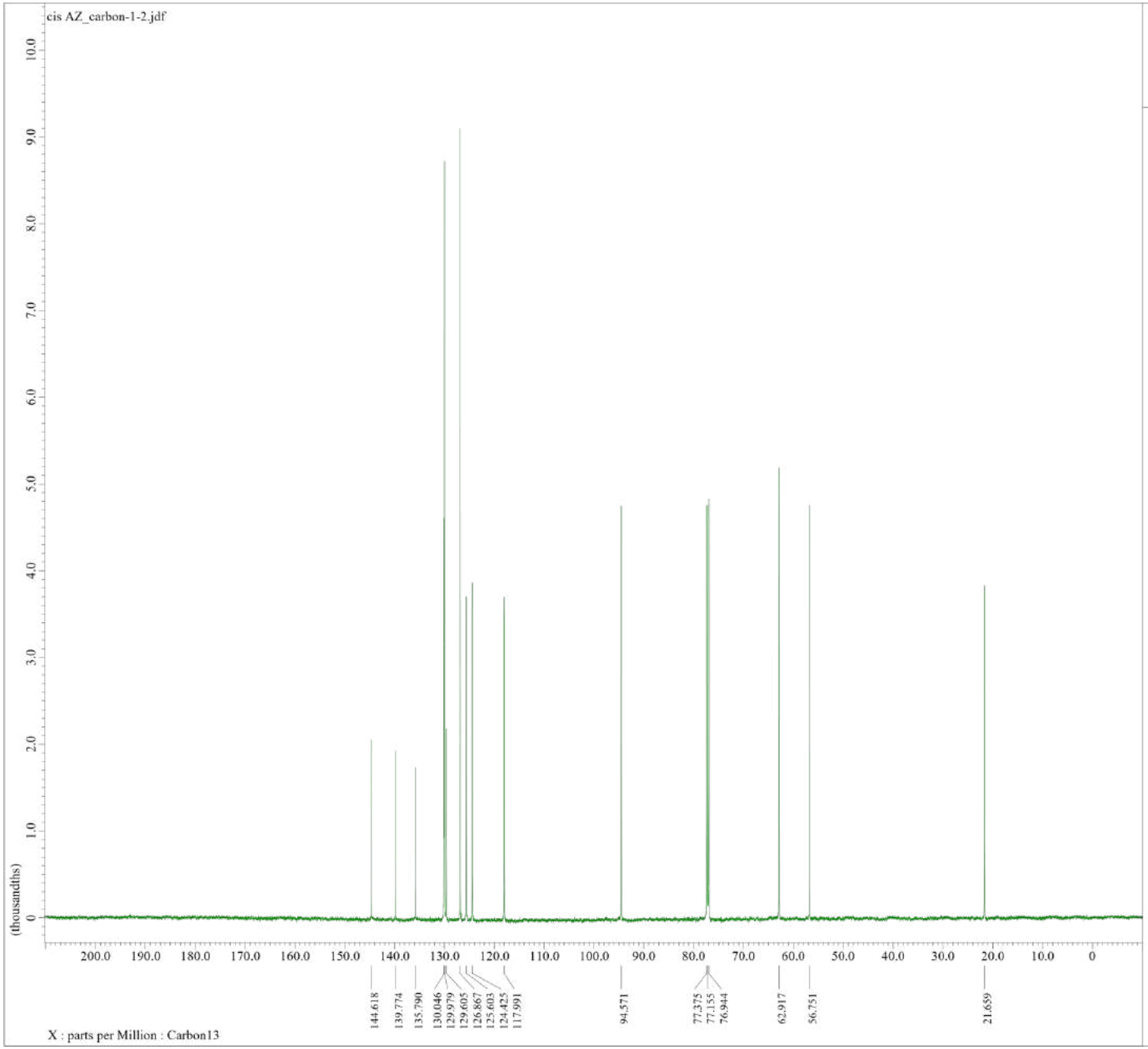
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 26
Temp_Get	= 19.6[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

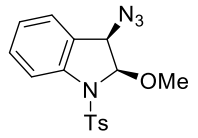


3a

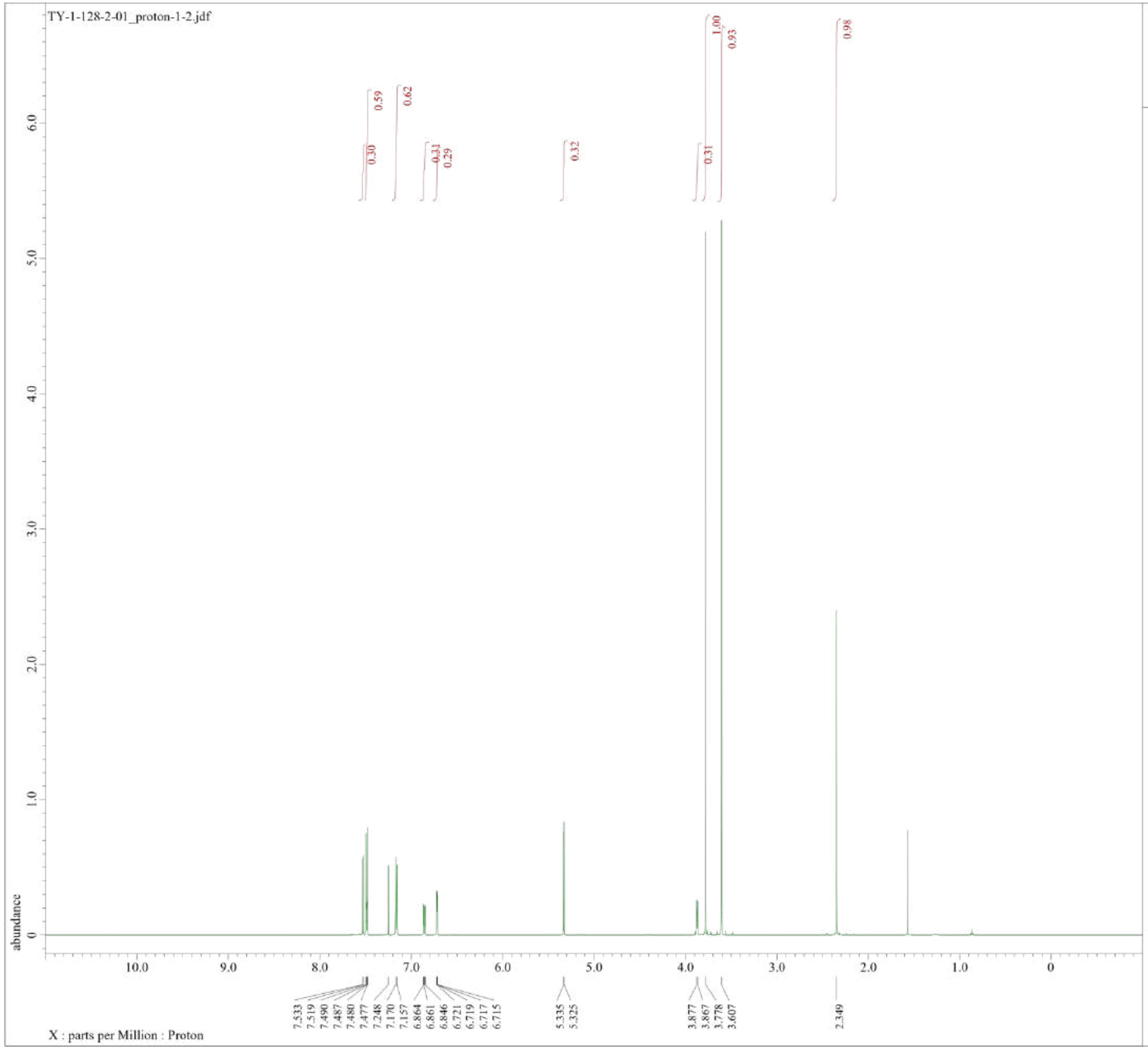


JEOL

Filename	= cis AZ_carbon-1-2.
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= cis AZ
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-APR-2021 15:21:
Revision_Time	= 24-APR-2021 15:53:
Comment	= cis AZIN
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15[us]
Clipped	= TRUE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 19.9[dC]
X_90_Width	= 8.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 2.93333333[us]
Irr_Atn_Dec	= 26.162[dB]
Irr_Atn_Dec_Calc	= 26.162[dB]
Irr_Atn_Dec_Default_Calc	= 26.162[dB]
Irr_Atn_Noe	= 26.162[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



3a



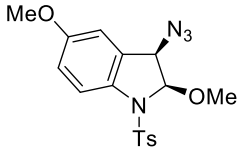
JEOL

```
Filename              = TY-1-128-2-01_proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-1-128-2-01
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 10-JUN-2021 22:36:00
Revision_Time         = 14-JUN-2021 10:22:57

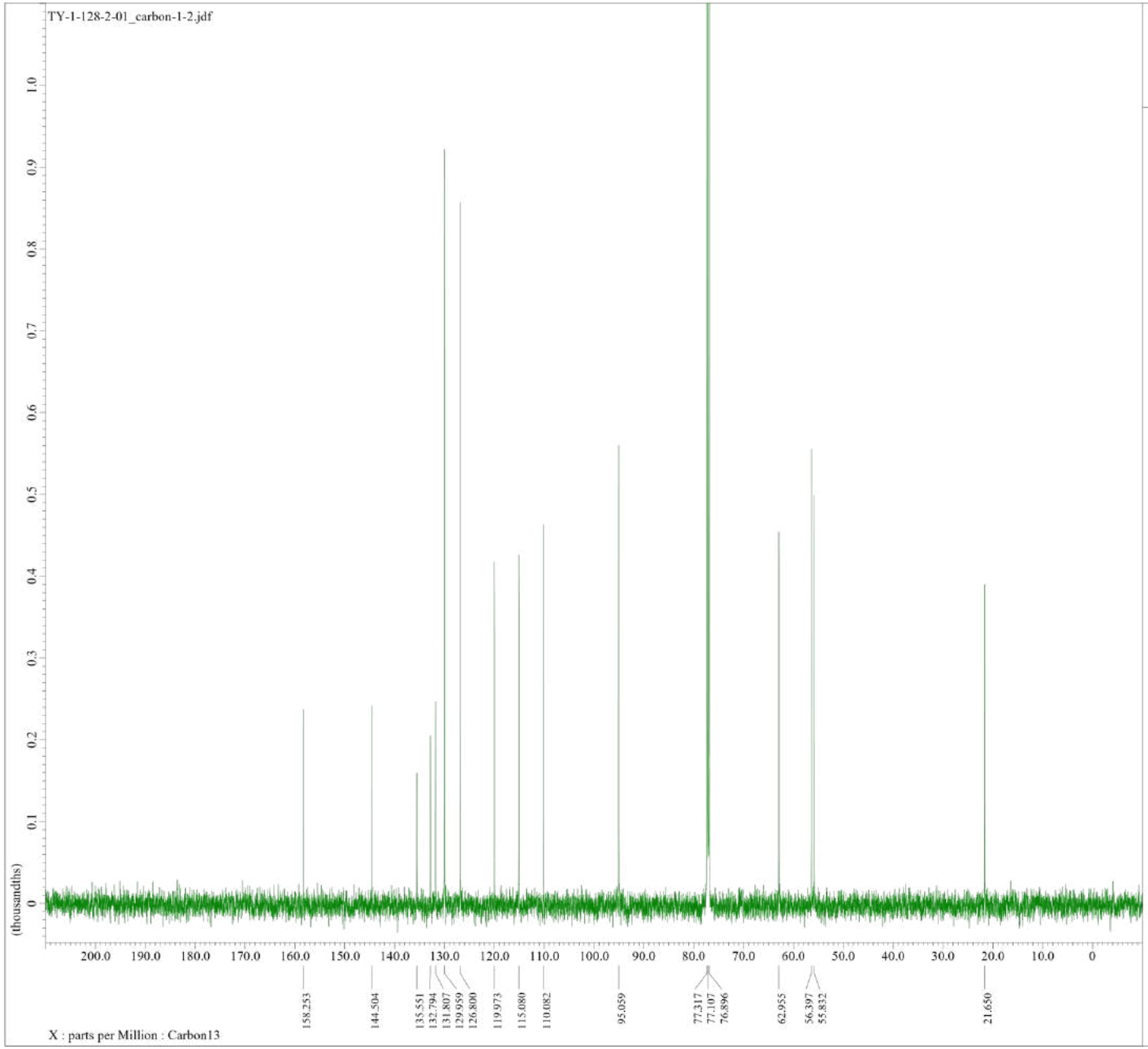
Comment               = 5-OMe A2
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 46
Temp_Get              = 20.7[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

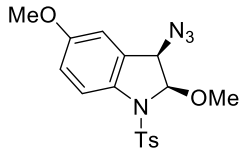


3b

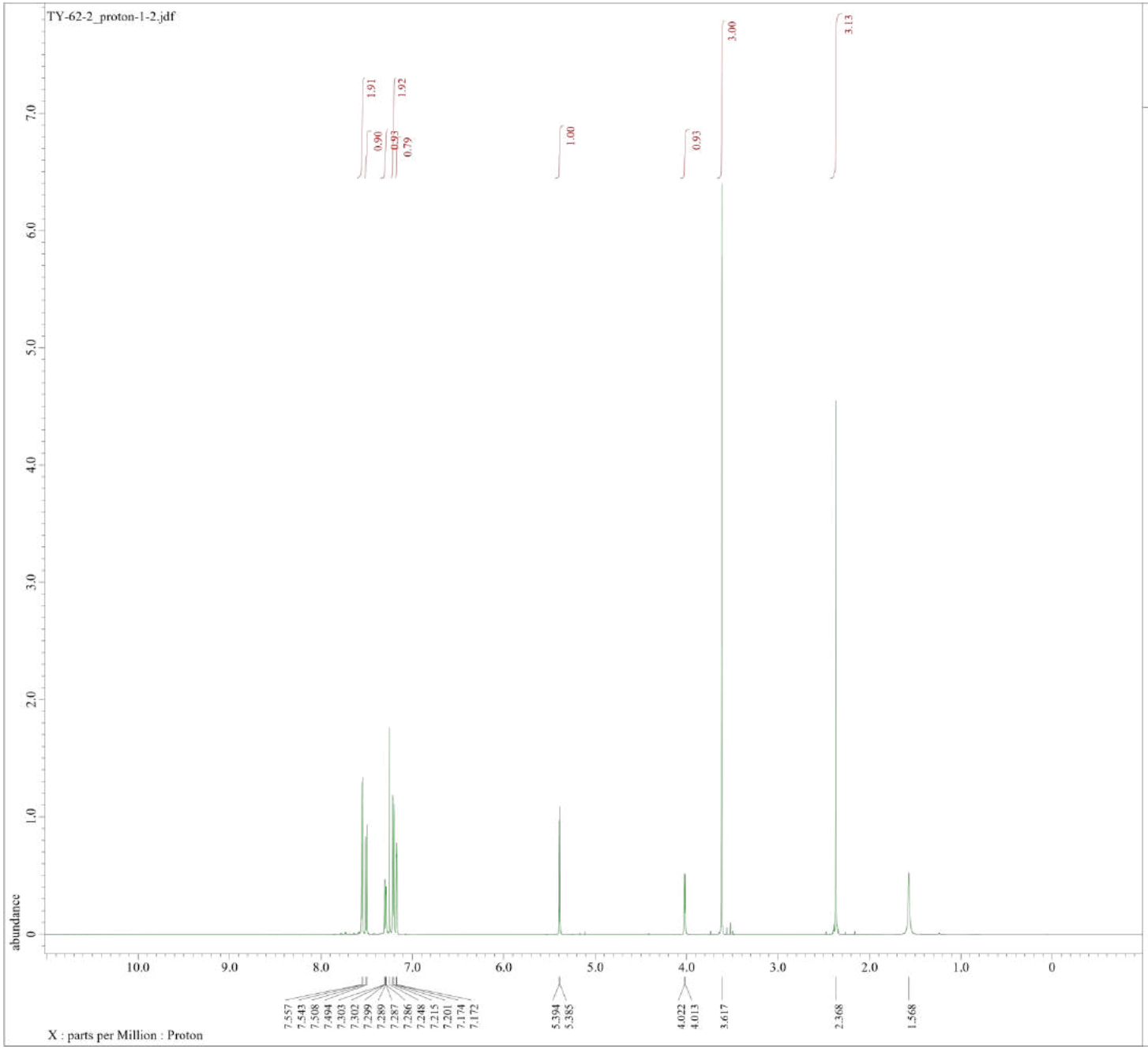


JEOL

Filename	= TY-1-128-2-01_carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-1-128-2-01
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-JUN-2021 22:37:
Revision_Time	= 14-JUN-2021 10:25:
Comment	= 5-OMe AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



3b



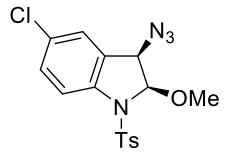
JEOL

```
Filename              = TY-62-2_proton-1-2.jd
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-62-2
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 18-MAY-2021 16:43:58
Revision_Time         = 18-MAY-2021 17:18:45

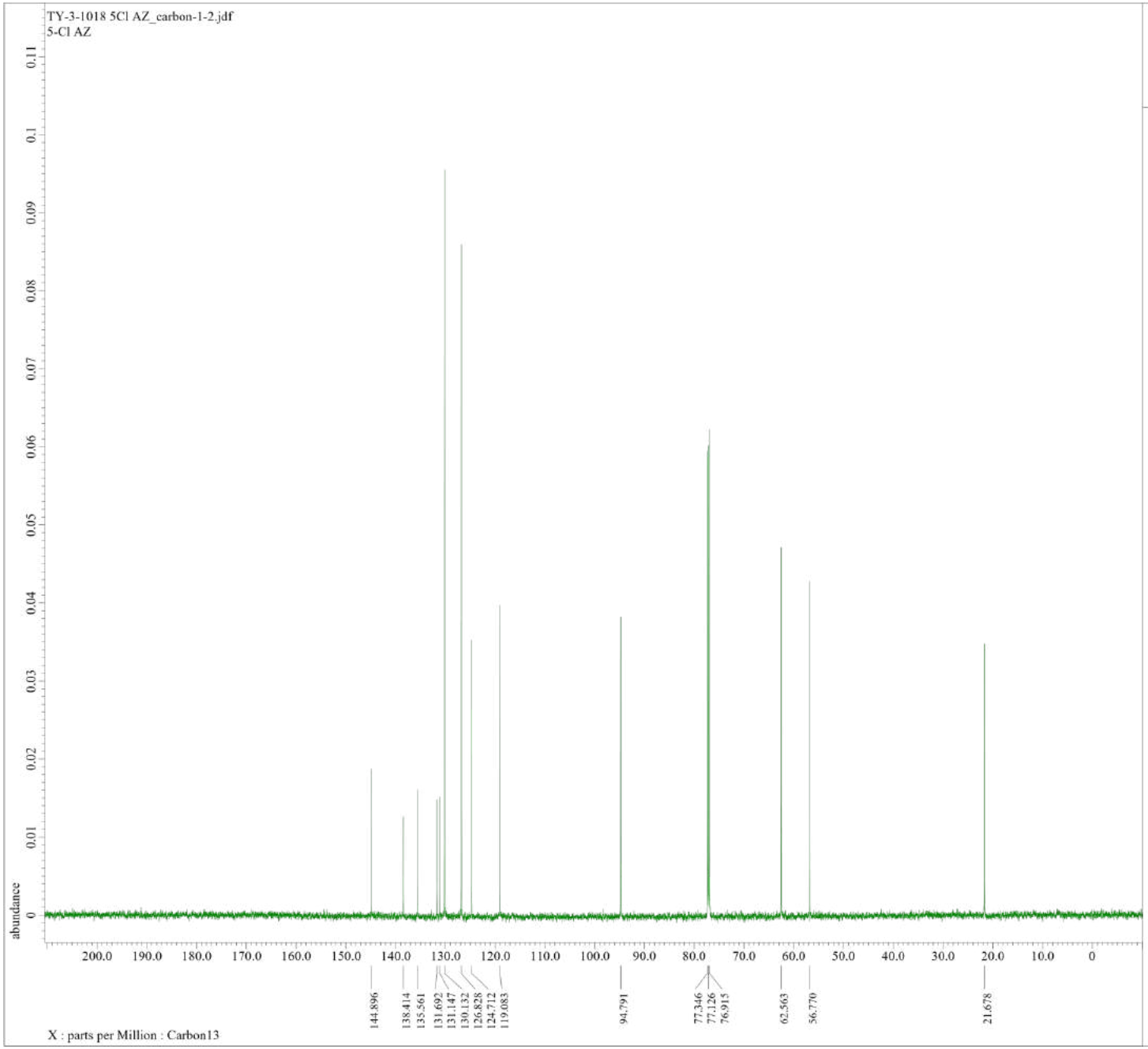
Comment               = 5-Cl AZIN
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 5[us]
Clipped               = TRUE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 20[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 4.75[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

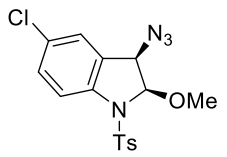


3c

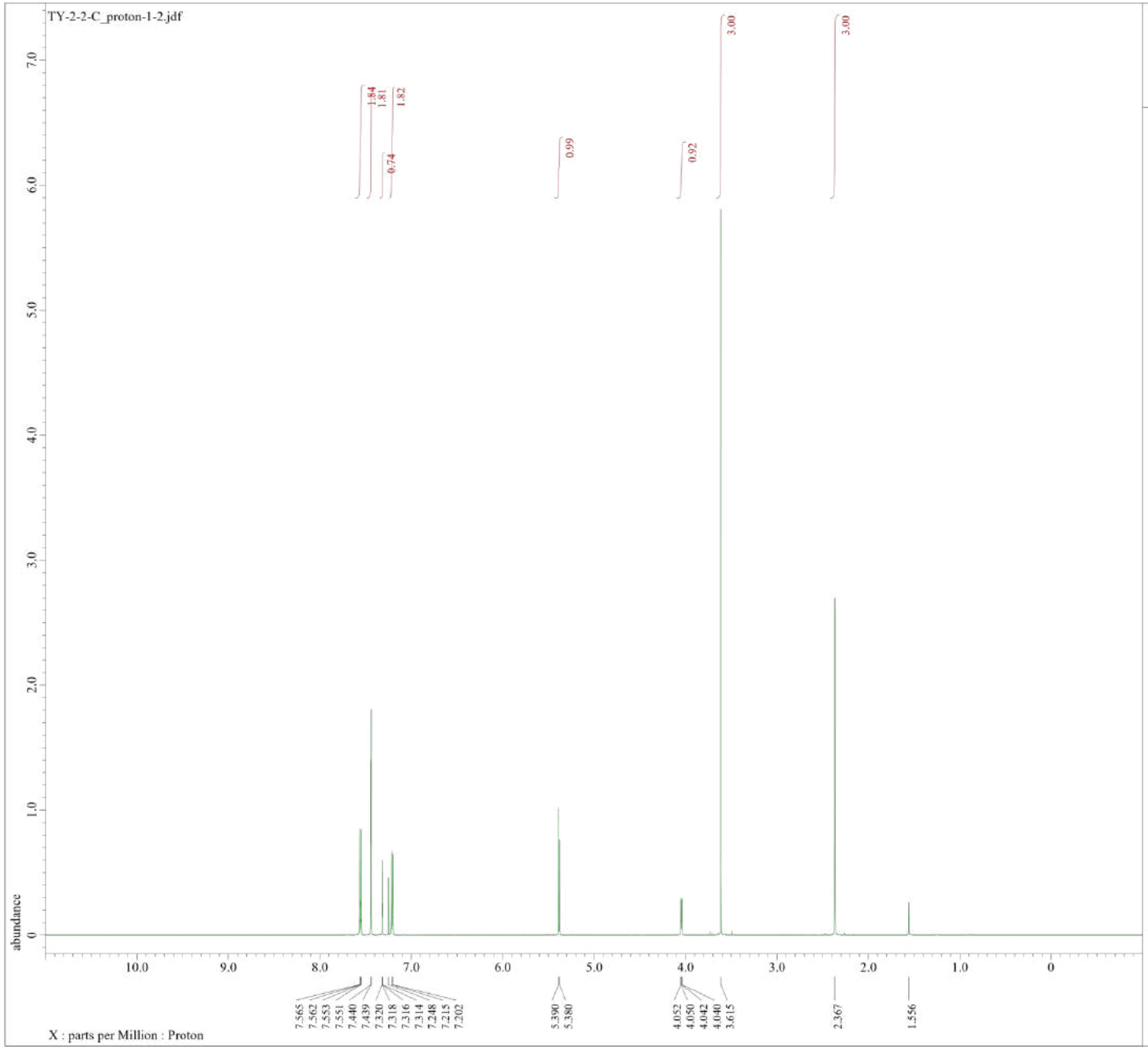


JEOL

Filename	= TY-3-1018 5Cl AZ_c
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-3-1018 5Cl AZ
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-OCT-2021 21:21:
Revision_Time	= 18-OCT-2021 21:24:
Comment	= 5-Cl AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15[us]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[dC]
X_90_Width	= 9.6[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 3.2[us]
Irr_Atn_Dec	= 26.254[dB]
Irr_Atn_Dec_Calc	= 26.254[dB]
Irr_Atn_Dec_Default_Calc	= 26.254[dB]
Irr_Atn_Noe	= 26.254[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



3c



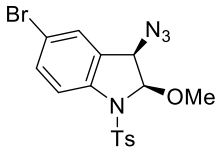
JEOL

```
Filename              = TY-2-2-C_proton-1-2.j
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-2-C
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 22-JUN-2021 15:09:21
Revision_Time         = 22-JUN-2021 15:29:33

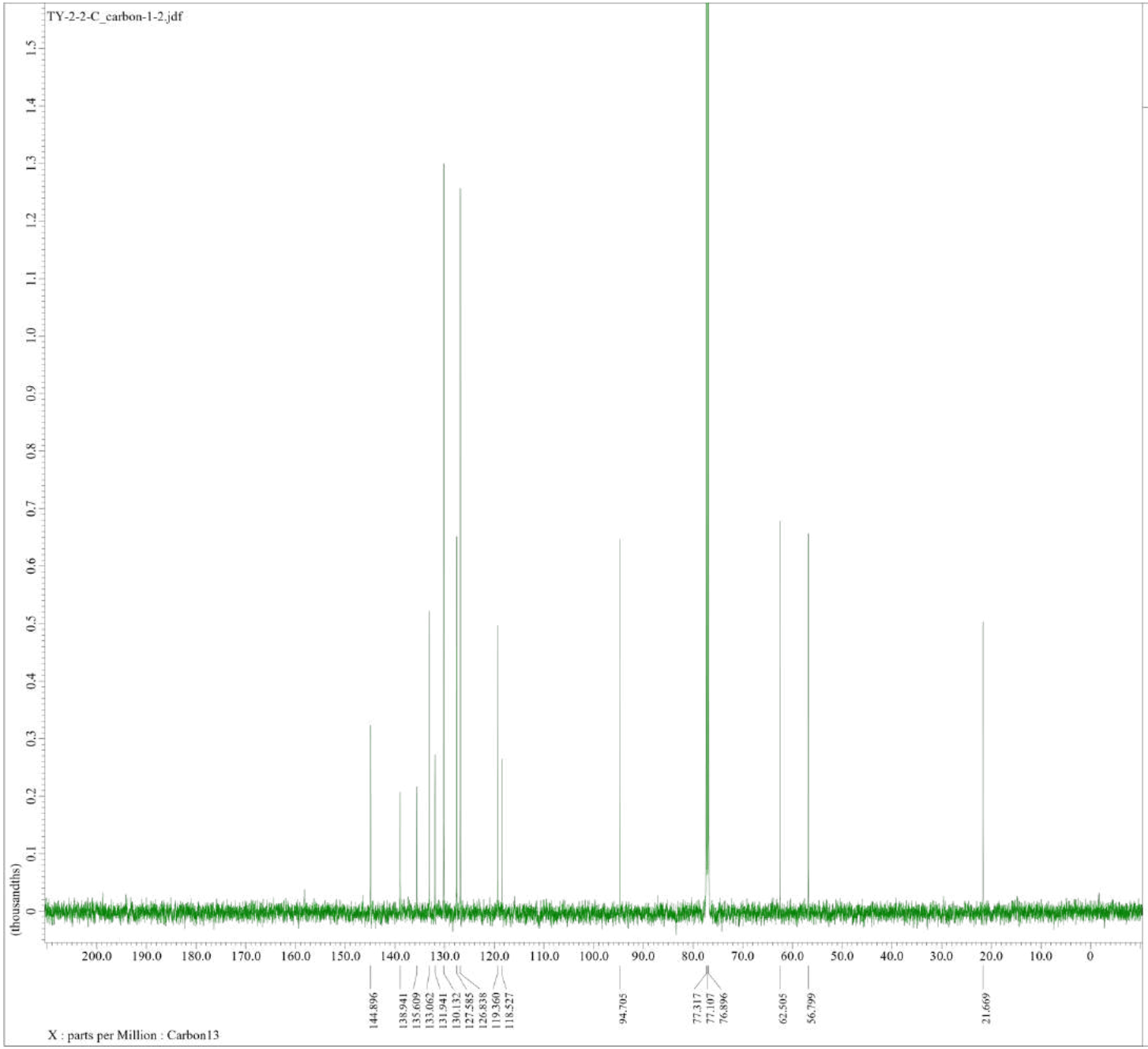
Comment               = 5-Br AZ
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 46
Temp_Get              = 20.8[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

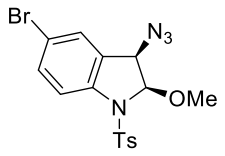


3d

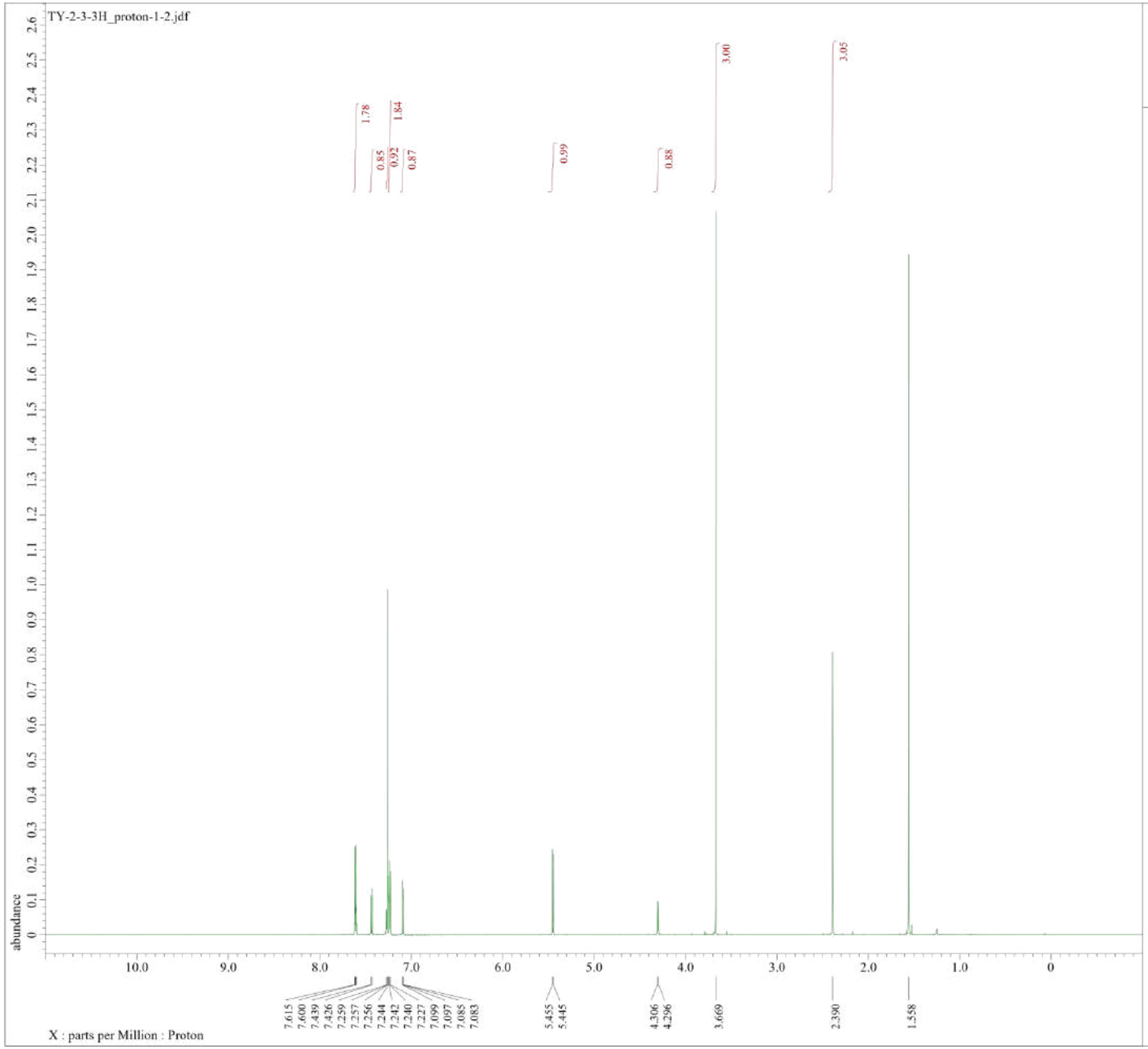


JEOL

Filename	= TY-2-2-C_carbon-1-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-2-C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JUN-2021 14:56:
Revision_Time	= 22-JUN-2021 15:32:
Comment	= 5-Br AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



3d



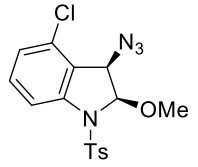
JEOL

```
Filename              = TY-2-3-3H_proton-1-2.
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-3-3H
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 21-JUN-2021 19:11:00
Revision_Time         = 21-JUN-2021 19:30:23

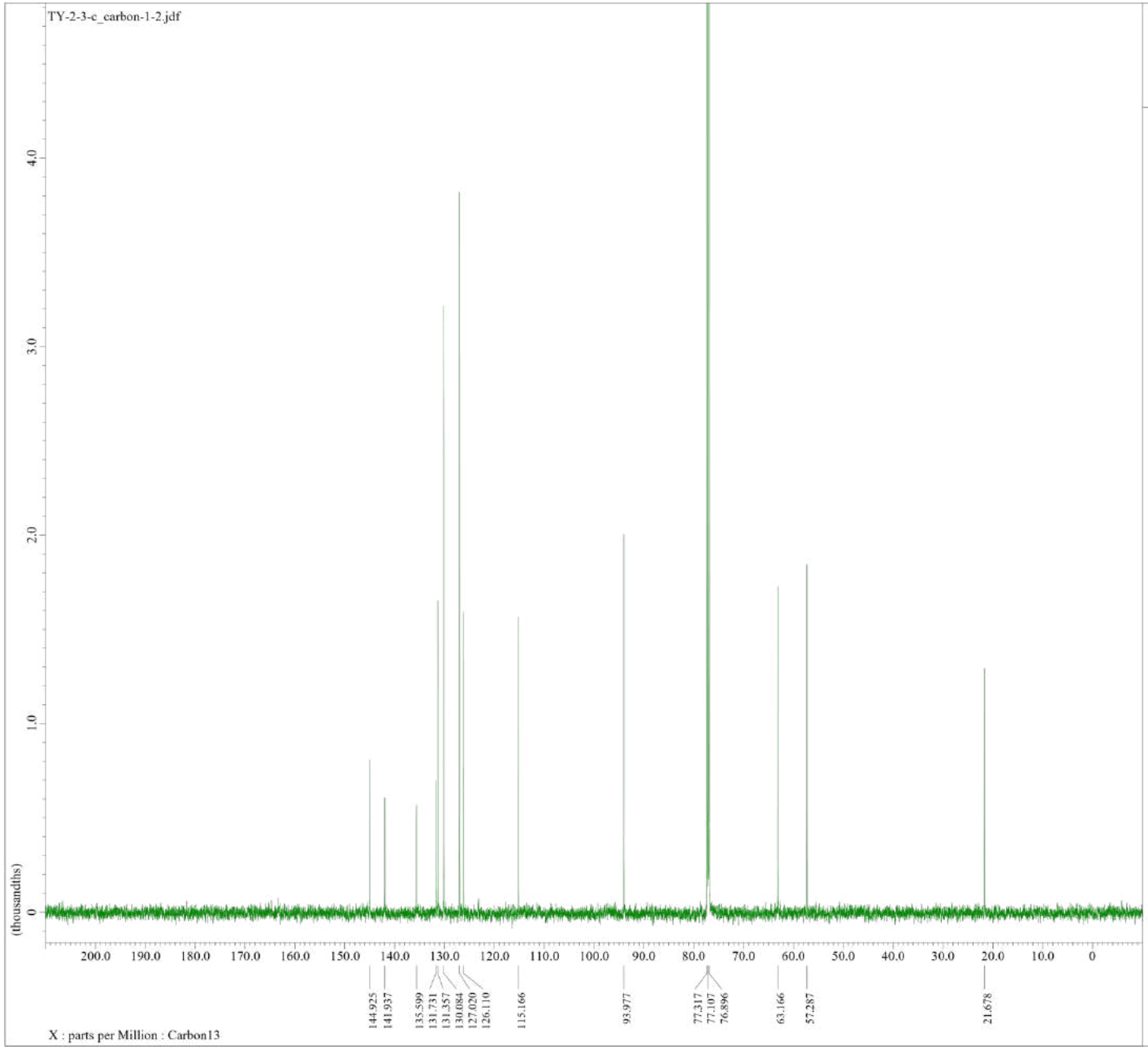
Comment               = 4-Cl AZ
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 20.7[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

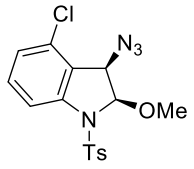


3e

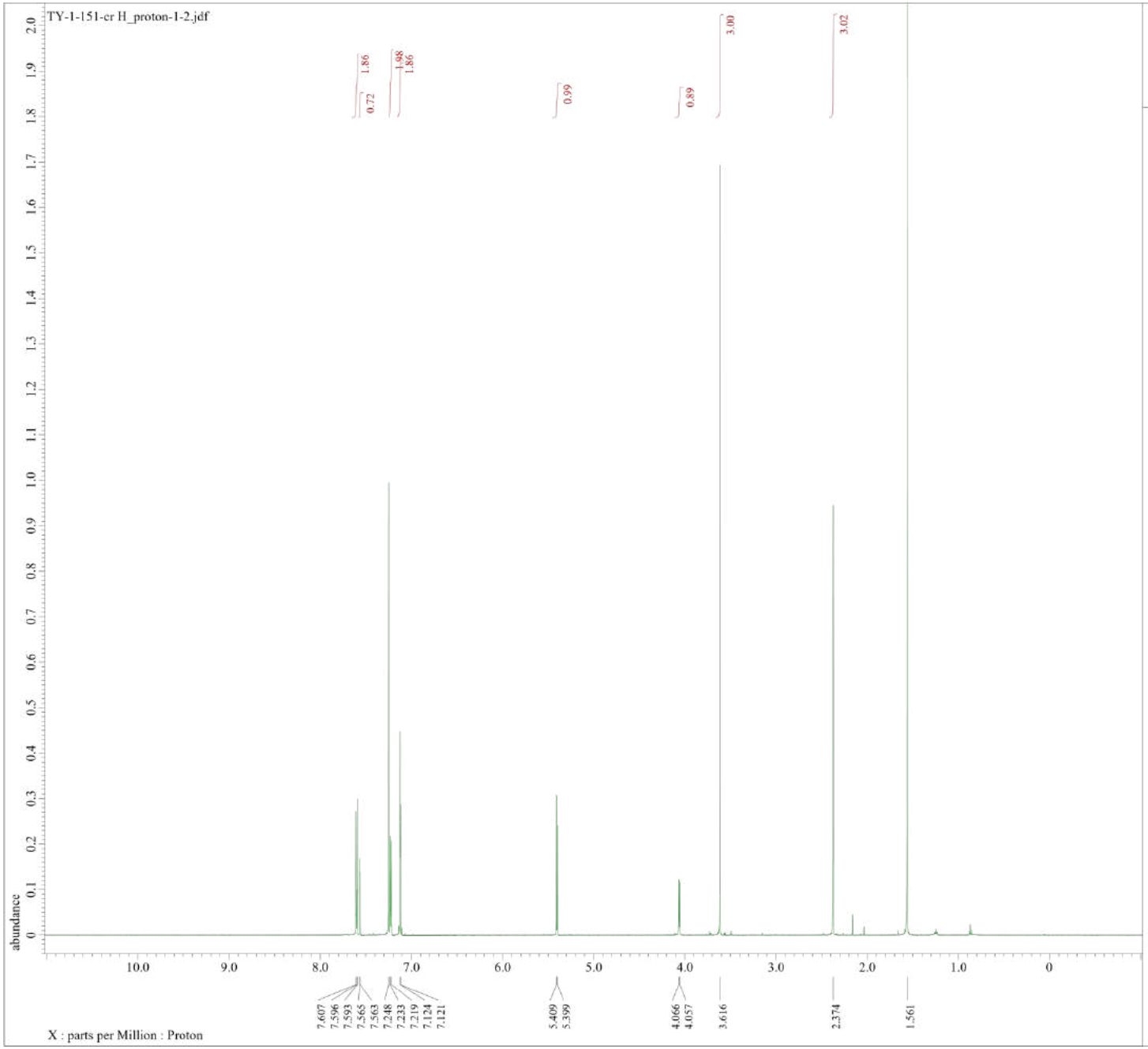


JEOL

Filename	= TY-2-3-c_carbon-1-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-3-c
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JUN-2021 15:37:
Revision_Time	= 22-JUN-2021 15:50:
Comment	= 4-Cl AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 385
Total_Scans	= 385
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]

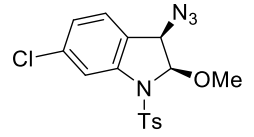


3e

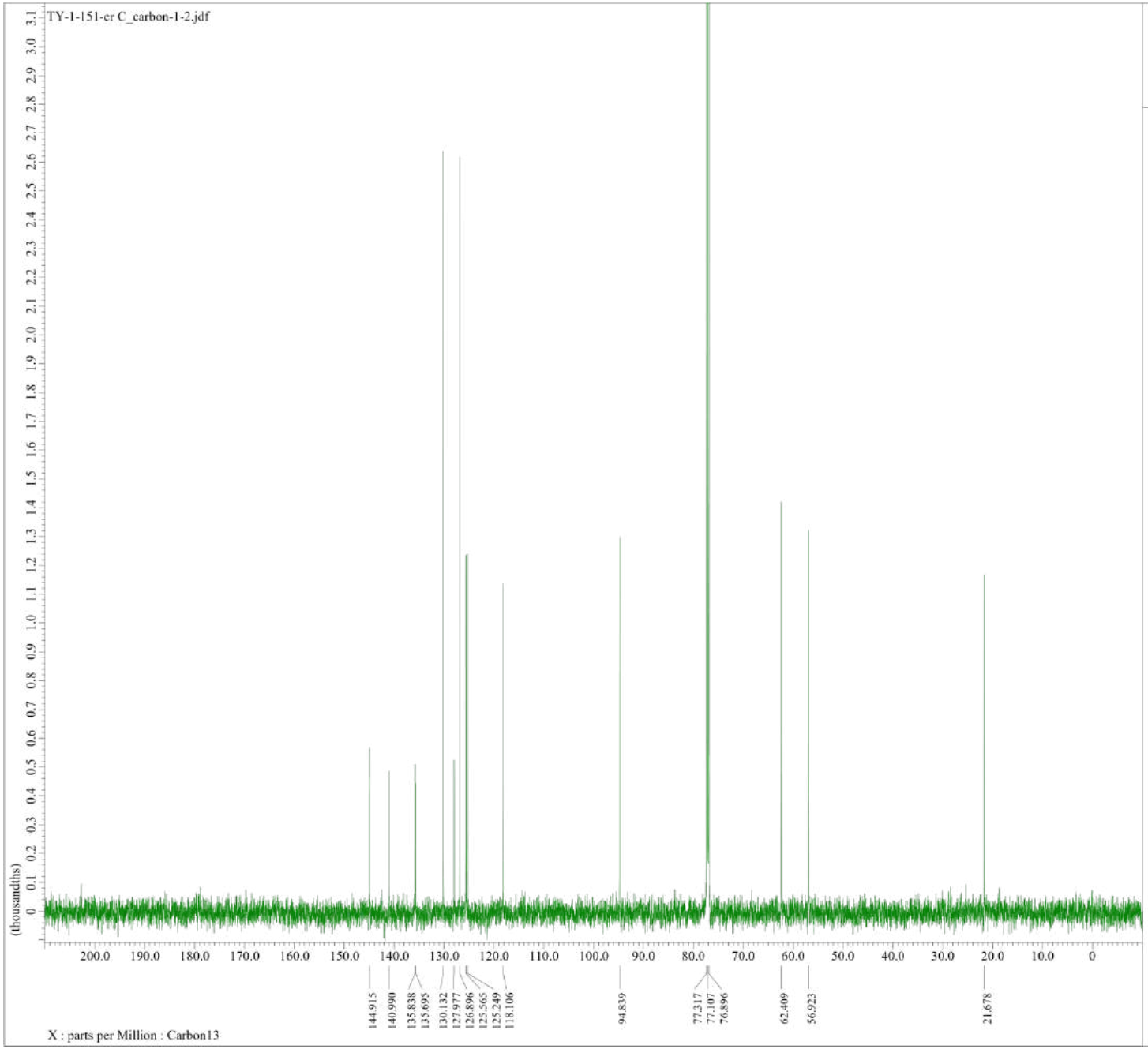


JEOL

Filename	= TY-1-151-cr H_proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-1-151-cr H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-JUN-2021 20:57:33
Revision_Time	= 17-JUN-2021 20:57:14
Comment	= 6-Cl AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.7[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

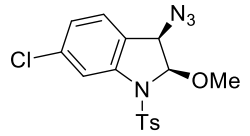


3f

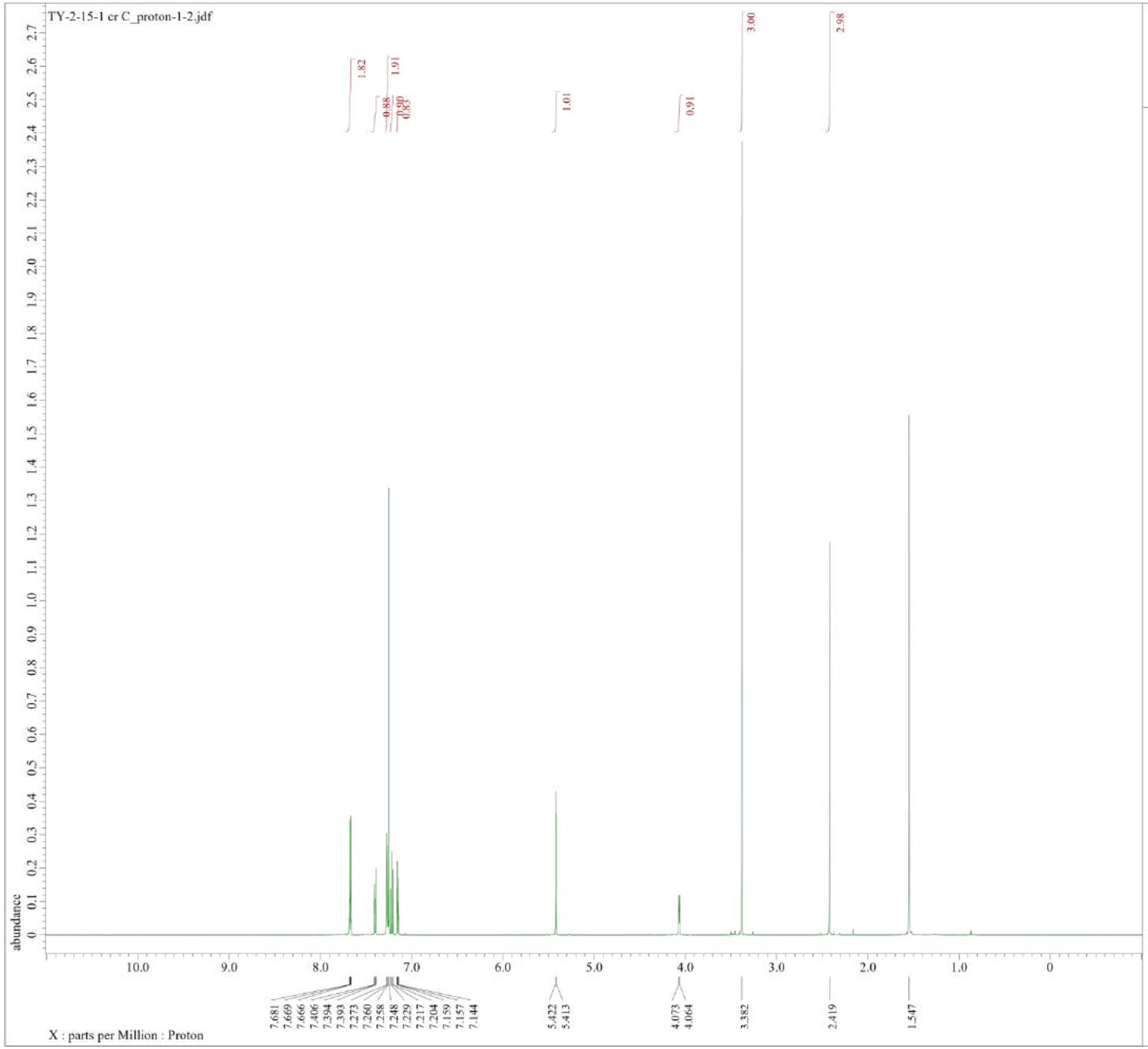


JEOL

Filename	= TY-1-151-cr C_carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-1-151-cr C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-JUN-2021 21:02:
Revision_Time	= 17-JUN-2021 21:10:
Comment	= 6-Cl AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



3f



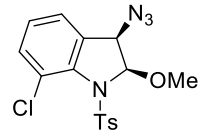
JEOL

```
Filename              = TY-2-15-1 cr C_proton
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-15-1 cr C
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 28-JUN-2021 16:20:12
Revision_Time         = 28-JUN-2021 16:27:19

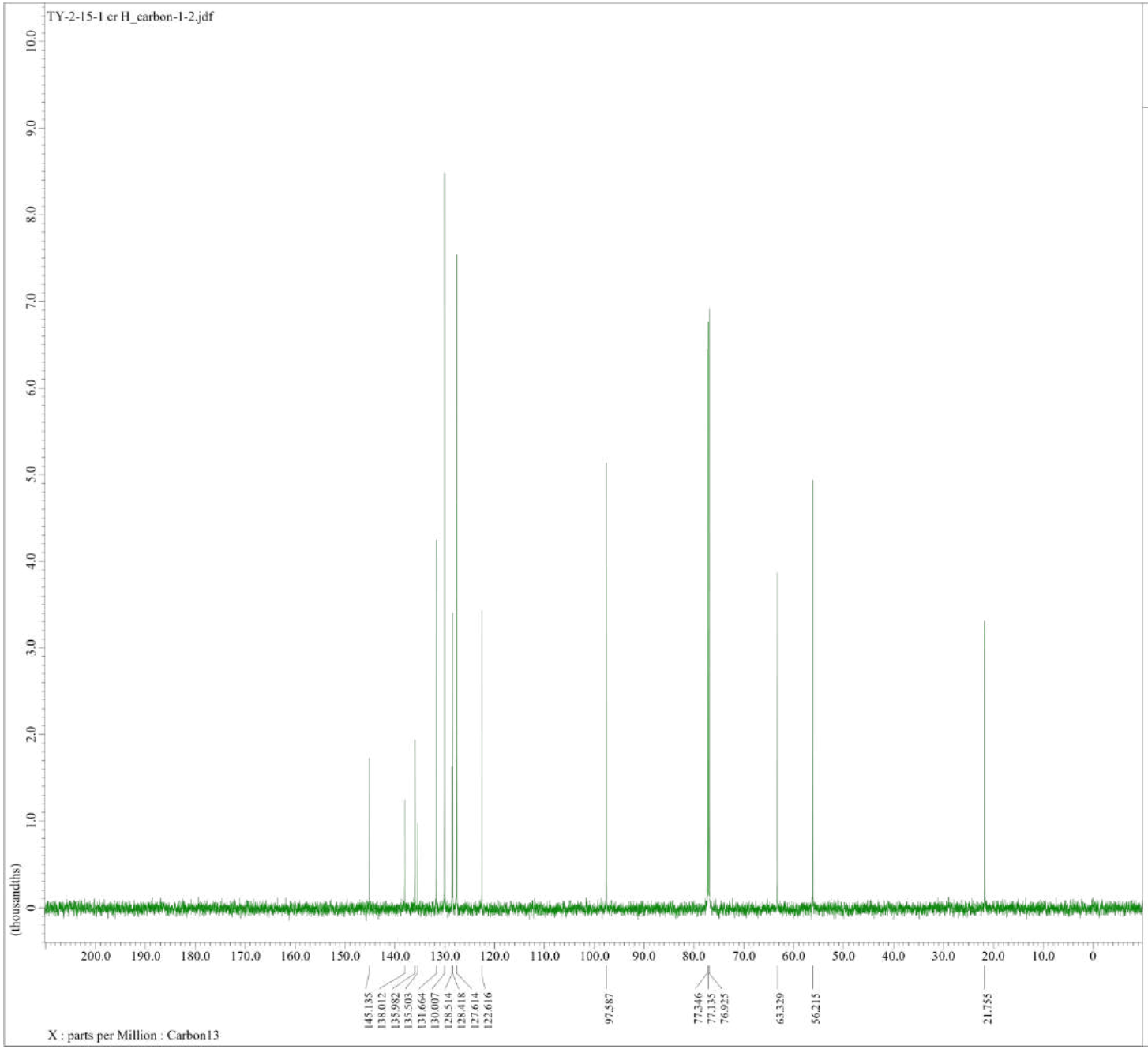
Comment               = 7-Cl AZ
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 20.8[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

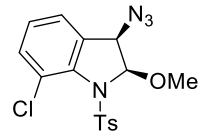


3g

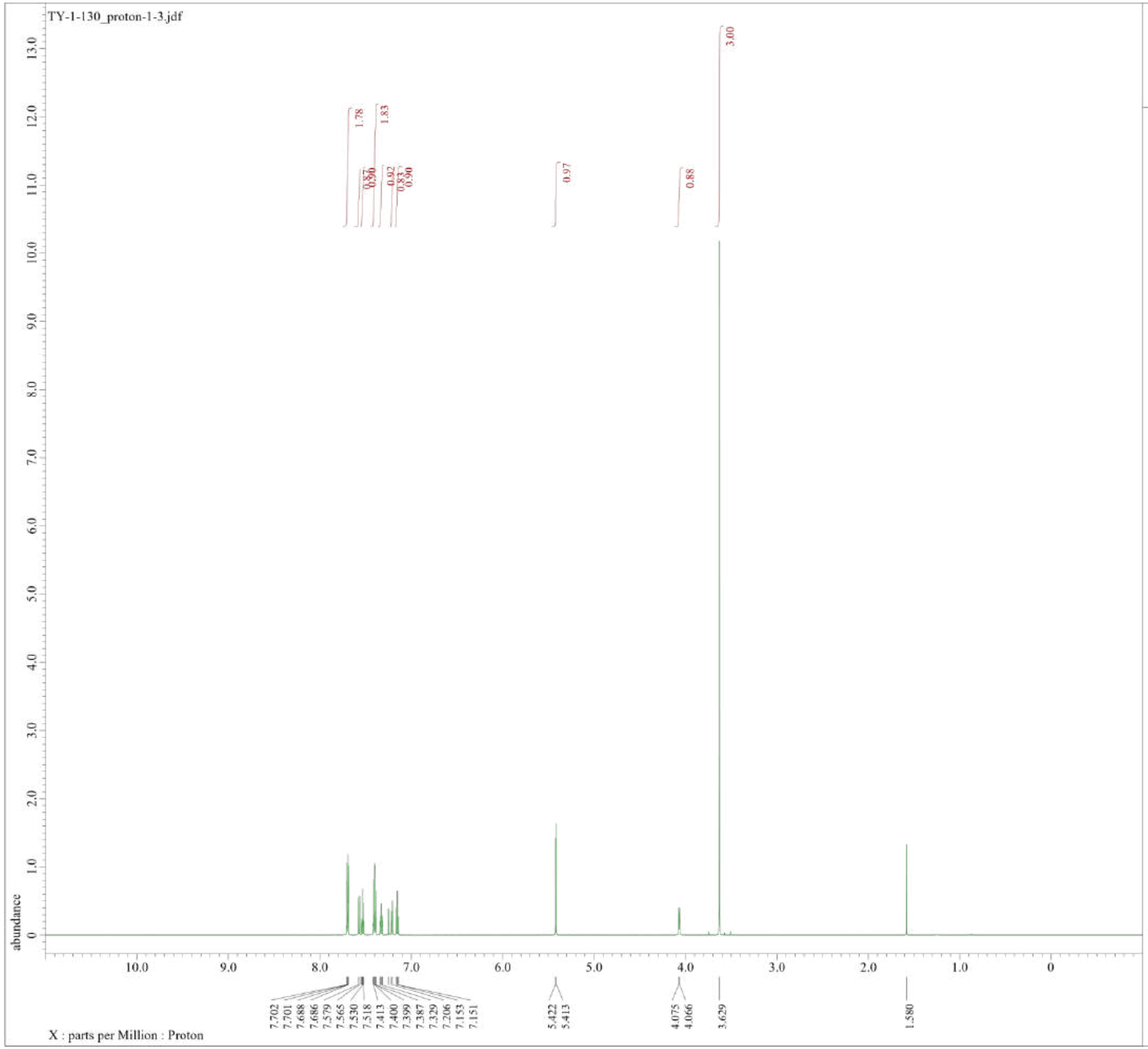


JEOL

Filename	= TY-2-15-1 cr H_car
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-15-1 cr H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-JUN-2021 16:26:
Revision_Time	= 28-JUN-2021 16:27:
Comment	= 7-Cl AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 108
Total_Scans	= 108
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



3g

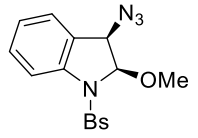



```
Filename              = TY-1-130_proton-1-3.j
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-1-130
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 10-JUN-2021 22:19:08
Revision_Time         = 14-JUN-2021 10:31:35

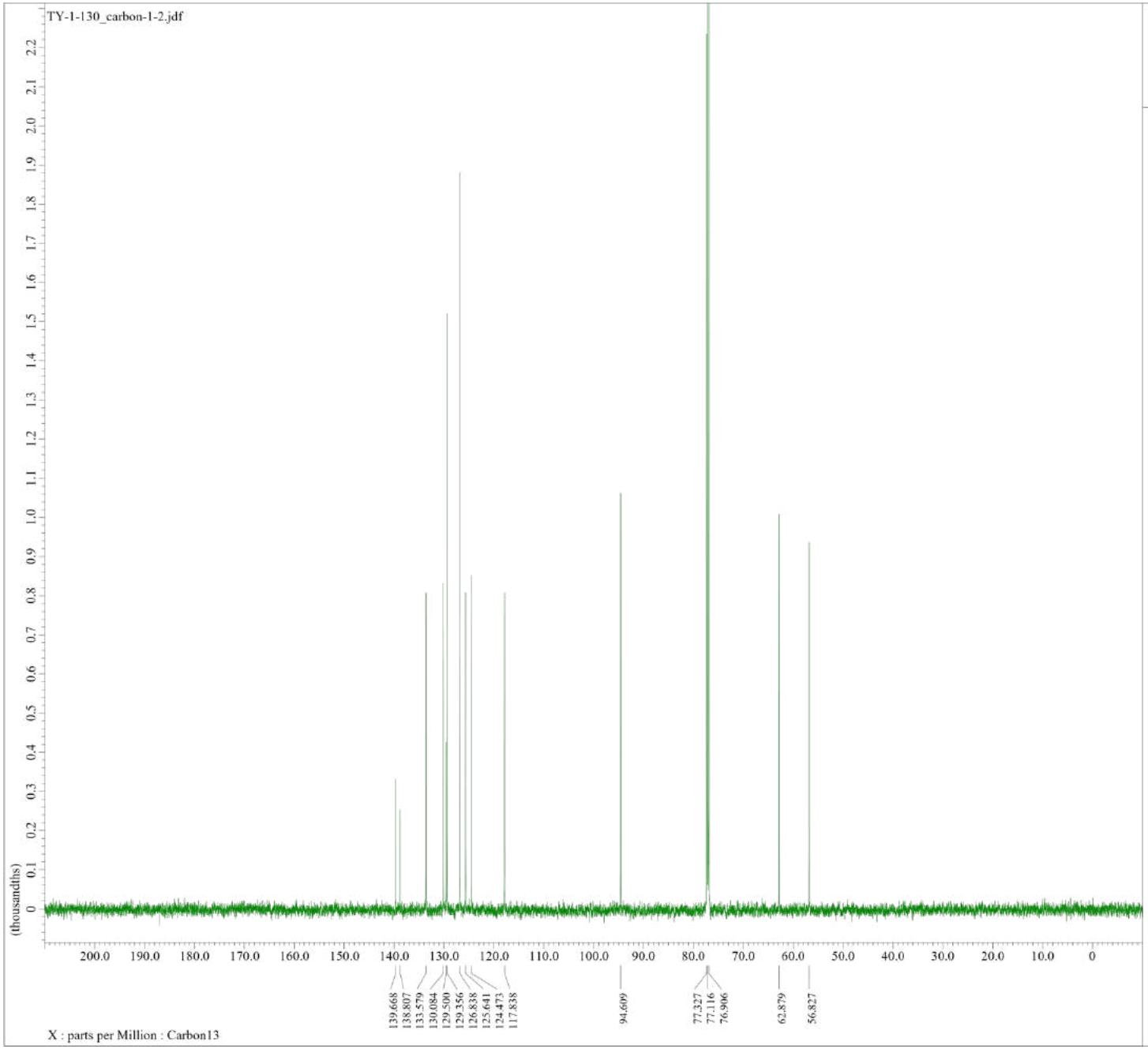
Comment               = Bs AE
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 46
Temp_Get              = 20.7[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

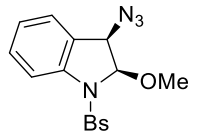


3h

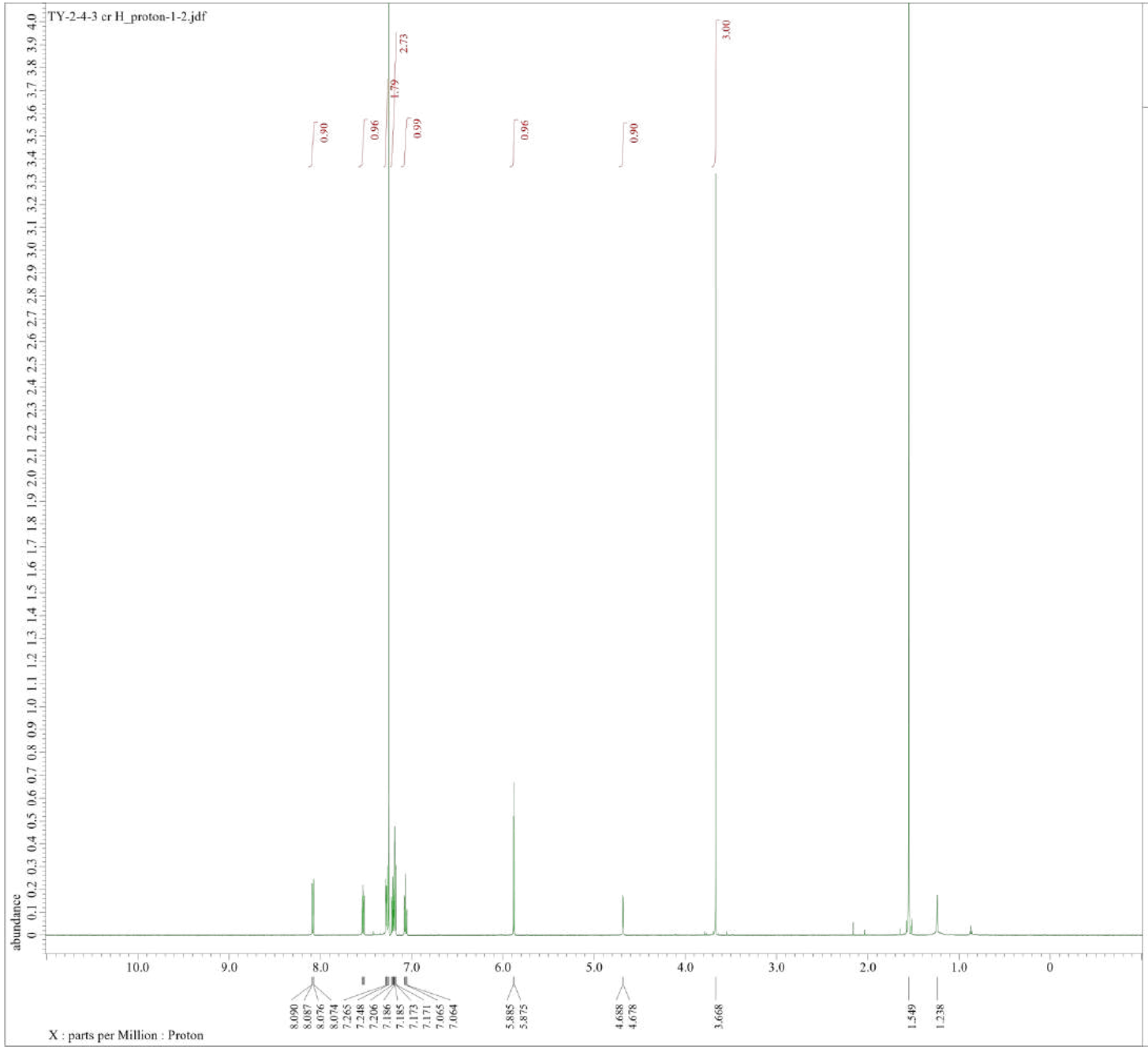


JEOL

Filename	= TY-1-130_carbon-1-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-1-130
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-JUN-2021 22:20:
Revision_Time	= 14-JUN-2021 10:32:
Comment	= Bs AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]

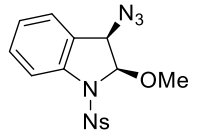


3h



JEOL

Filename	= TY-2-4-3 cr H_proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-4-3 cr H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-JUN-2021 16:08:40
Revision_Time	= 28-JUN-2021 16:09:10
Comment	= Ns AE
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 66
Temp_Get	= 20.8[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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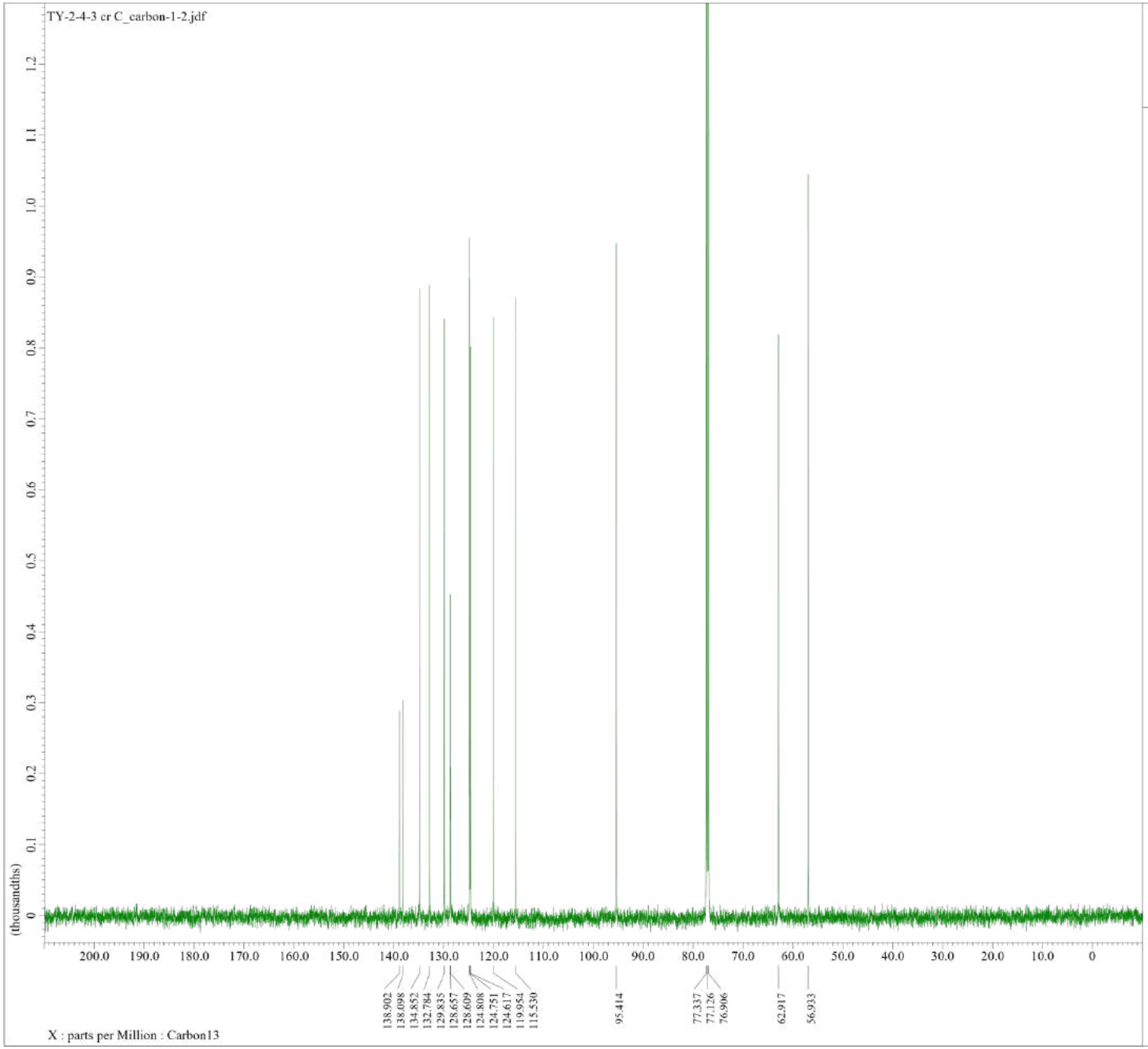
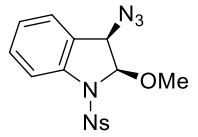


JEOL

Filename	= TY-2-4-3 cr C_carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-4-3 cr C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-JUN-2021 16:36:
Revision_Time	= 28-JUN-2021 16:55:
Comment	= Ns AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 513
Total_Scans	= 513
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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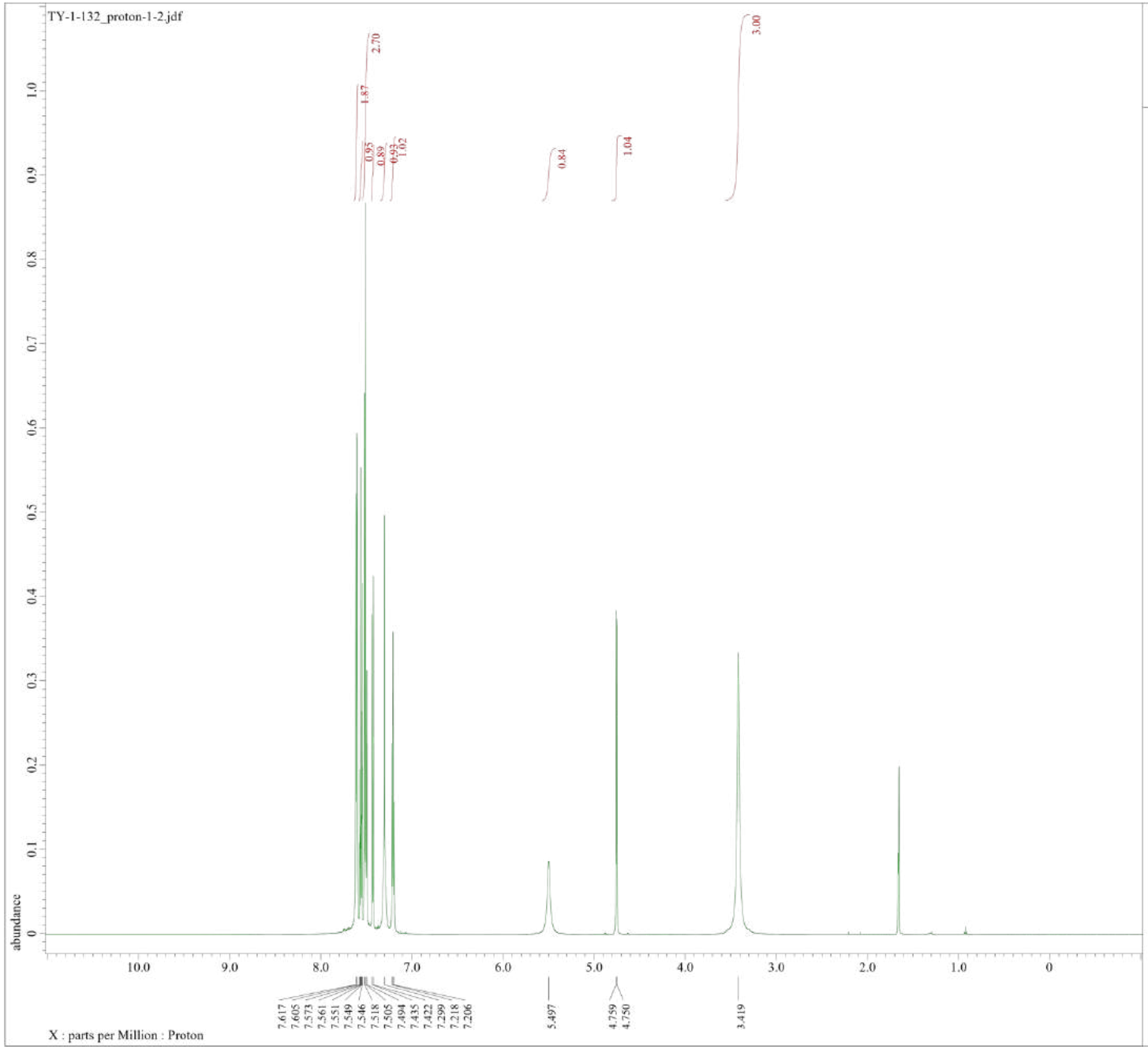
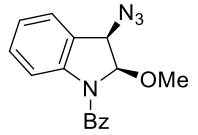


JEOL

Filename	= TY-1-132_proton-1-2.j
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-1-132
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-JUN-2021 21:44:34
Revision_Time	= 14-JUN-2021 10:46:11
Comment	= Bz AE
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 46
Temp_Get	= 20.7[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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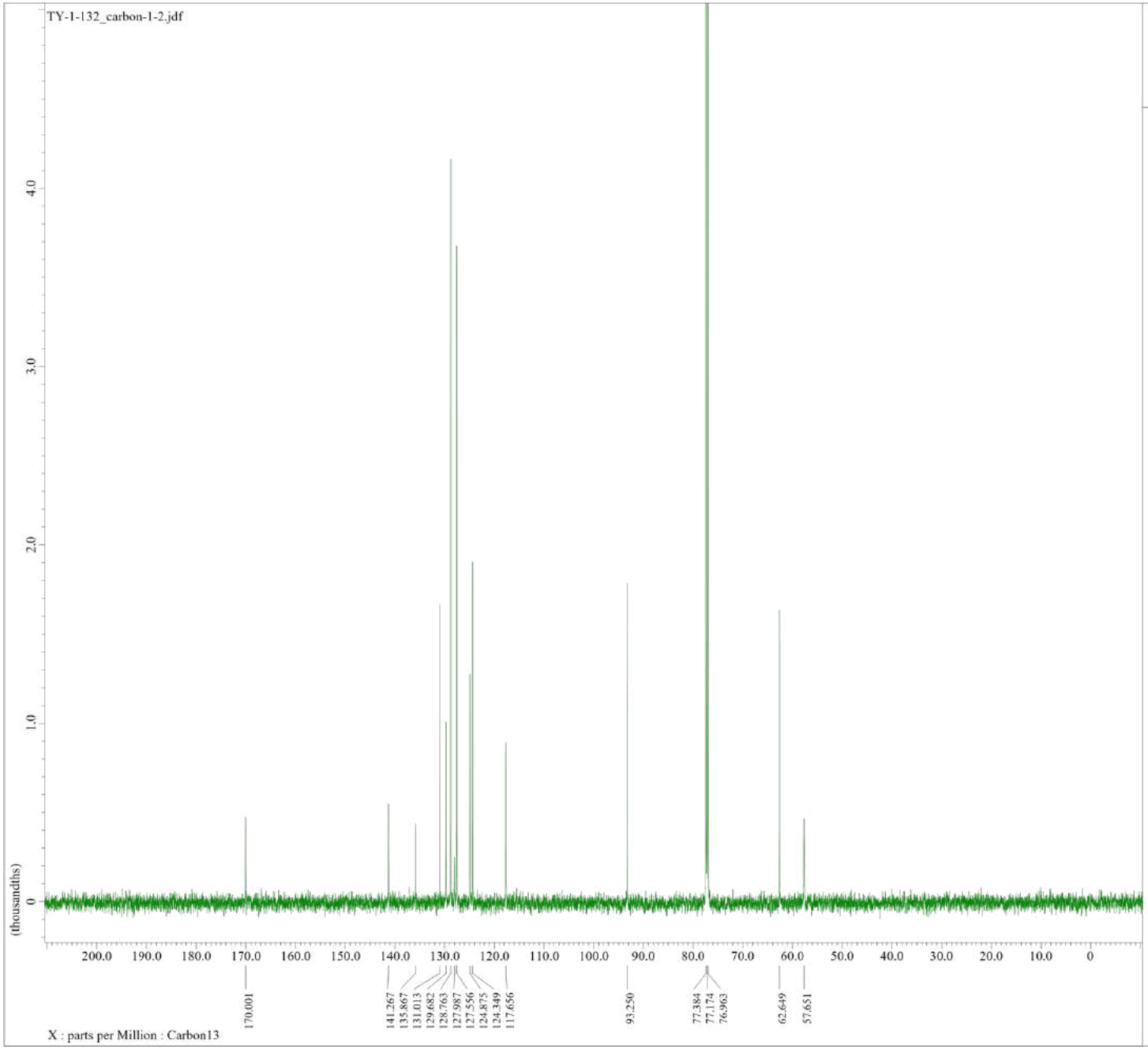
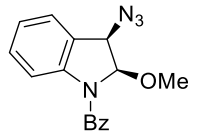



```
Filename                = TY-1-132_carbon-1-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = TY-1-132
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 10-JUN-2021 21:46:
Revision_Time           = 14-JUN-2021 10:49:

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

Field_Strength          = 14.09636928[T] (60
X_Acq_Duration          = 0.69206016[s]
X_Domain                = Carbon13
X_Freq                  = 150.91343039[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 1.44496109[Hz]
X_Sweep                 = 47.34848485[kHz]
X_Sweep_Clipped         = 37.87878788[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = TRUE
Scans                   = 256
Total_Scans             = 256

Relaxation_Delay        = 2[s]
Recvr_Gain              = 36
Temp_Get                = 20.8[dC]
X_90_Width              = 11.8[us]
X_Acq_Time              = 0.69206016[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.6[dB]
X_Pulse                 = 3.93333333[us]
Irr_Atn_Dec             = 27.986[dB]
Irr_Atn_Dec_Calc        = 27.986[dB]
Irr_Atn_Dec_Default_Calc = 27.986[dB]
Irr_Atn_Noe             = 27.986[dB]
Irr_Dec_Bandwidth_Hz    = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm   = 12.05794078[ppm]
Irr_Dec_Freq            = 600.1723046[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 76[us]
Irr_Pwidth_Default      = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1        = 76[us]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
Experiment_Path         = c:\Program Files\J
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]
```



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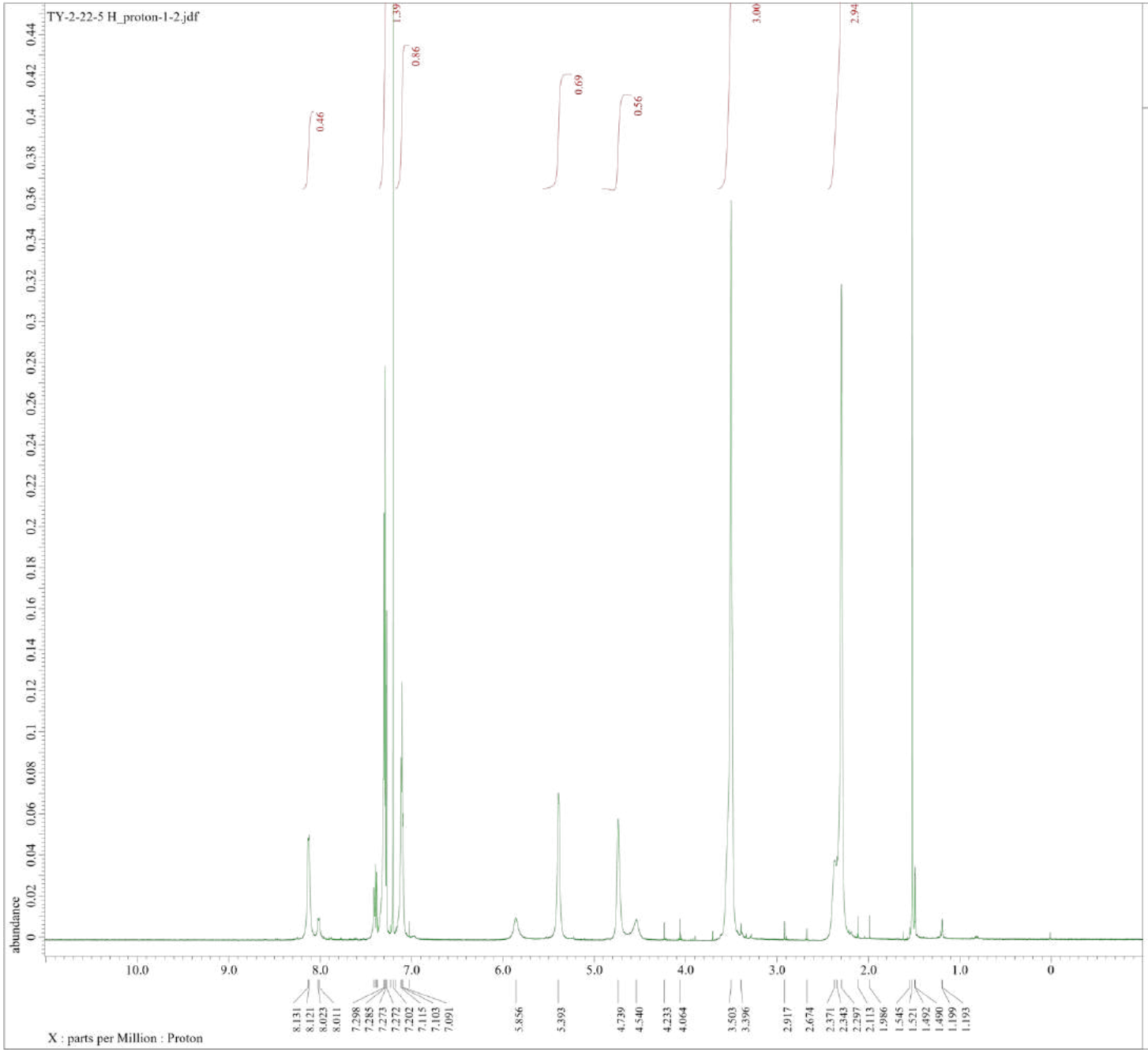
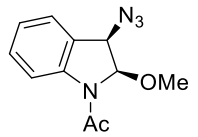
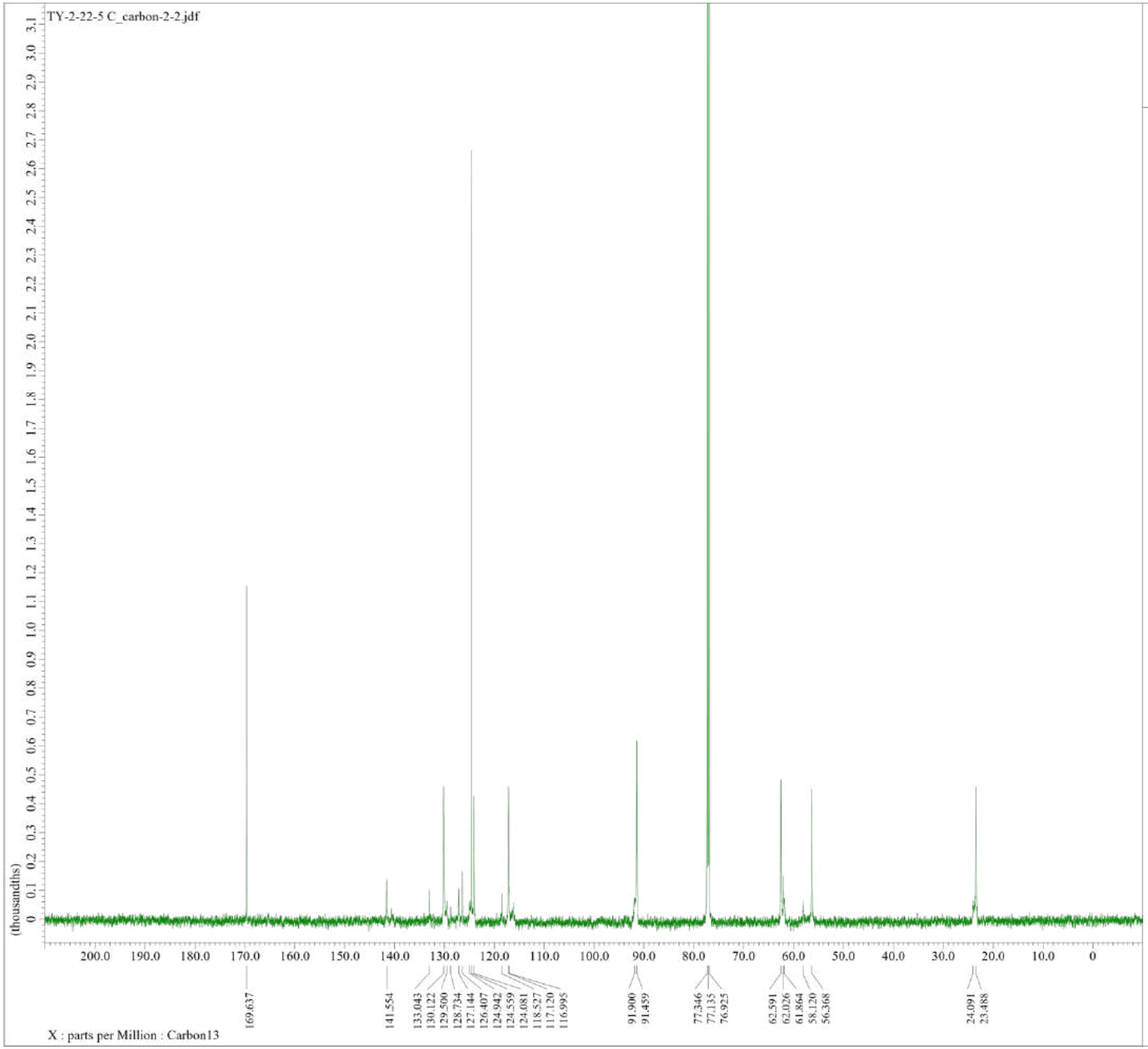


JEOL

Filename	= TY-2-22-5 H_proton-1-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-22-5 H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2021 14:14:37
Revision_Time	= 25-JUN-2021 16:58:02
Comment	= Ac AE
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.6[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

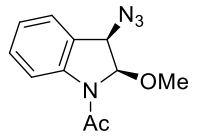


3k



JEOL

Filename	= TY-2-22-5 C_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-22-5 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2021 15:31:
Revision_Time	= 25-JUN-2021 17:01:
Comment	= Ac AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1776
Total_Scans	= 1776
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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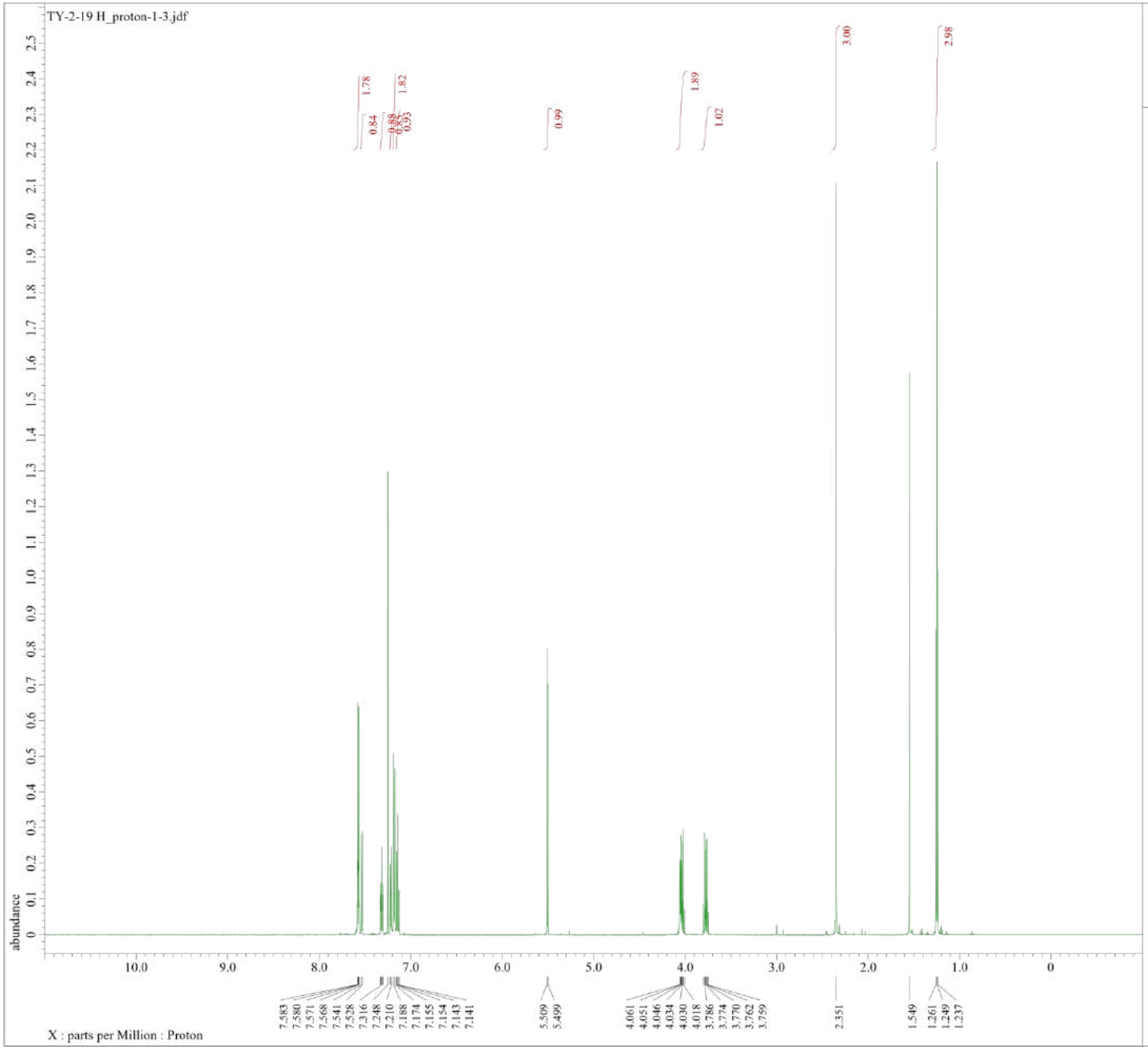
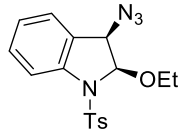
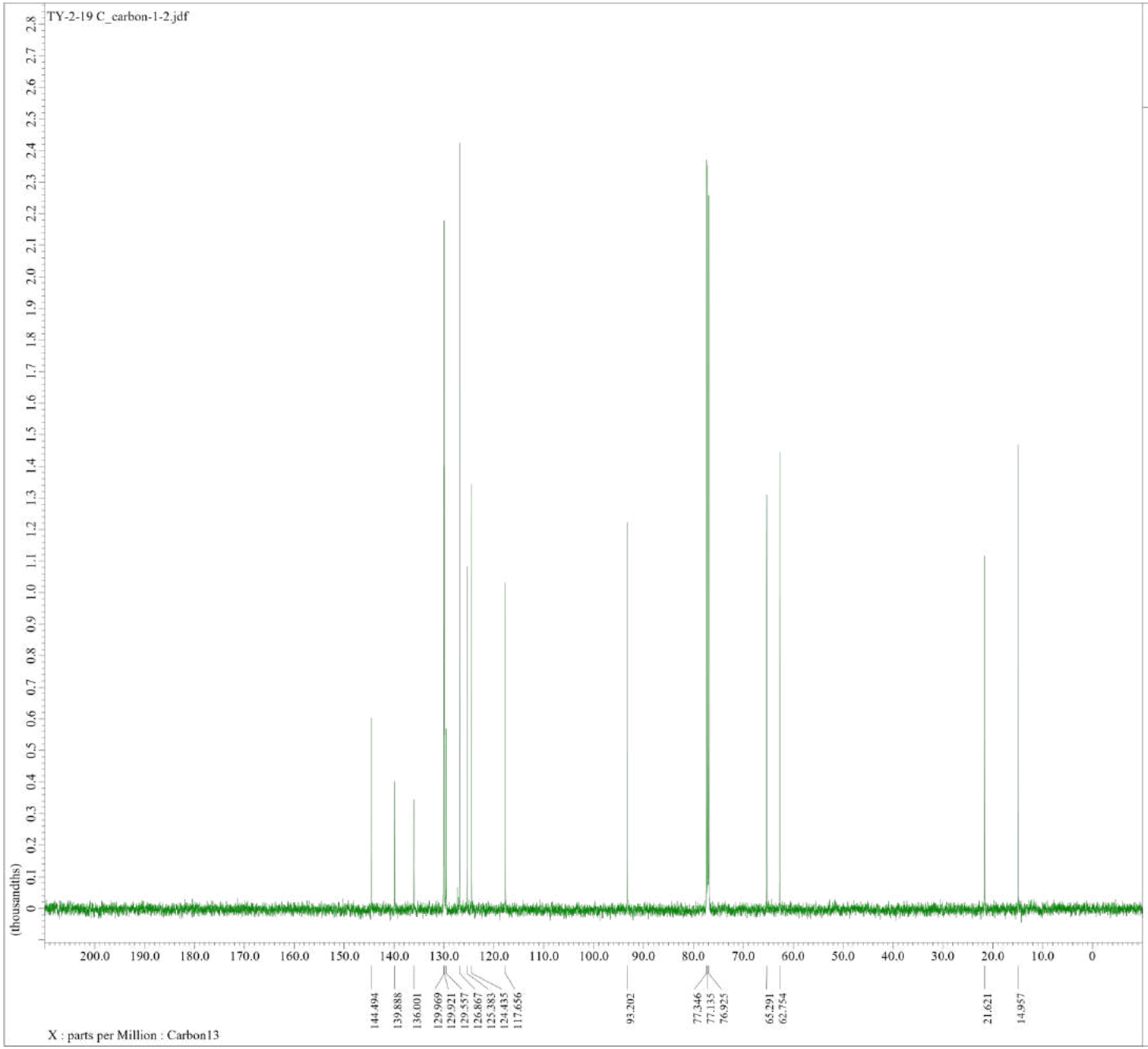


JEOL

Filename	= TY-2-19 H_proton-1-3.
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-19 H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2021 14:39:09
Revision_Time	= 25-JUN-2021 16:52:23
Comment	= 2-OEt AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

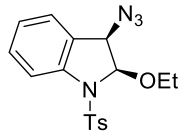


3l



JEOL

Filename	= TY-2-19 C_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-19 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUN-2021 14:45:
Revision_Time	= 25-JUN-2021 16:53:
Comment	= 2-OEt AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 178
Total_Scans	= 178
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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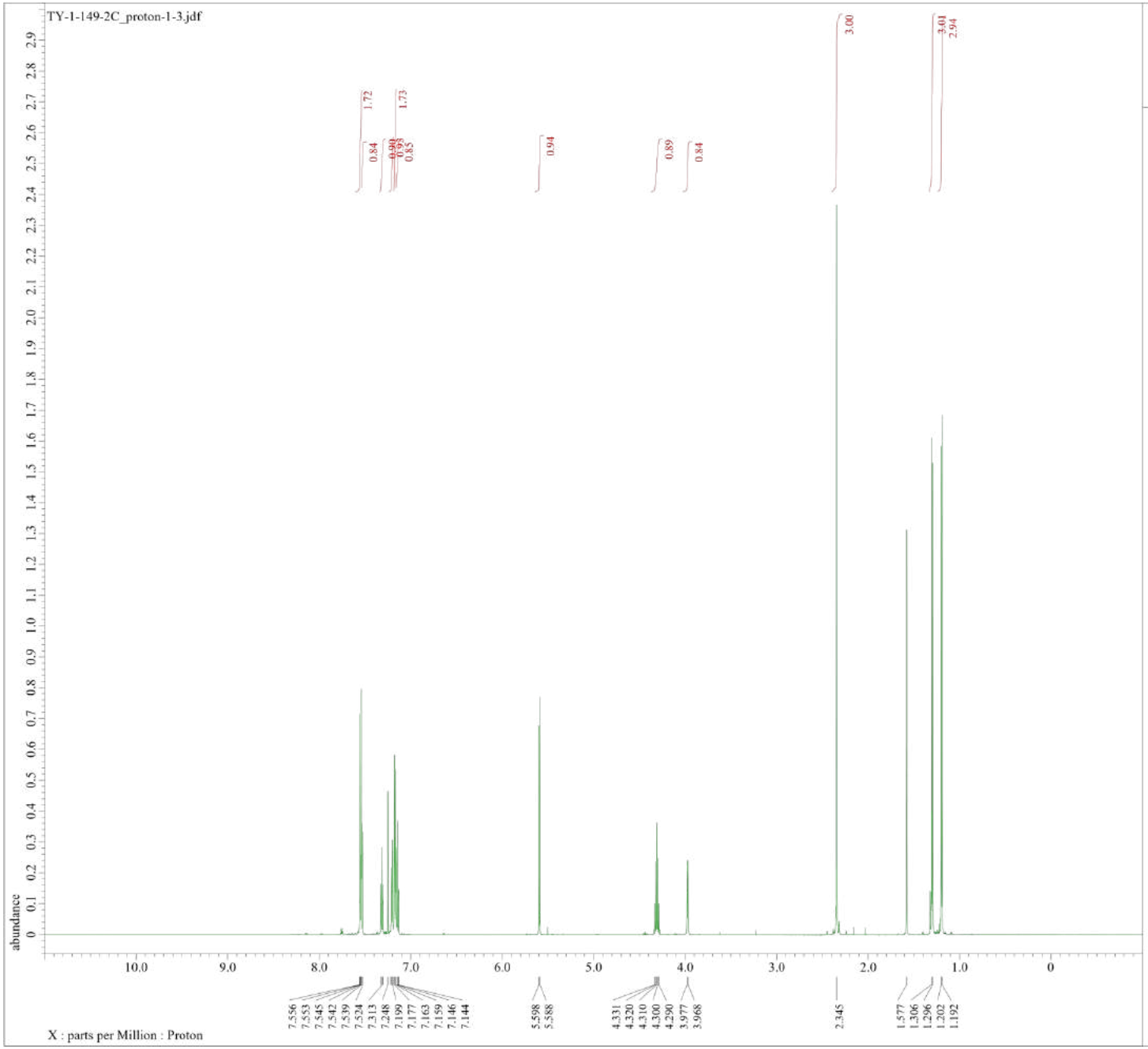
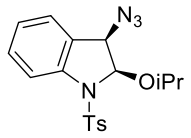


JEOL

Filename	= TY-1-149-2C_proton-1-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-1-149-2C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-JUN-2021 15:43:44
Revision_Time	= 17-JUN-2021 15:54:50
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 4
Total_Scans	= 4
Relaxation_Delay	= 1[s]
Recvr_Gain	= 46
Temp_Get	= 20.7[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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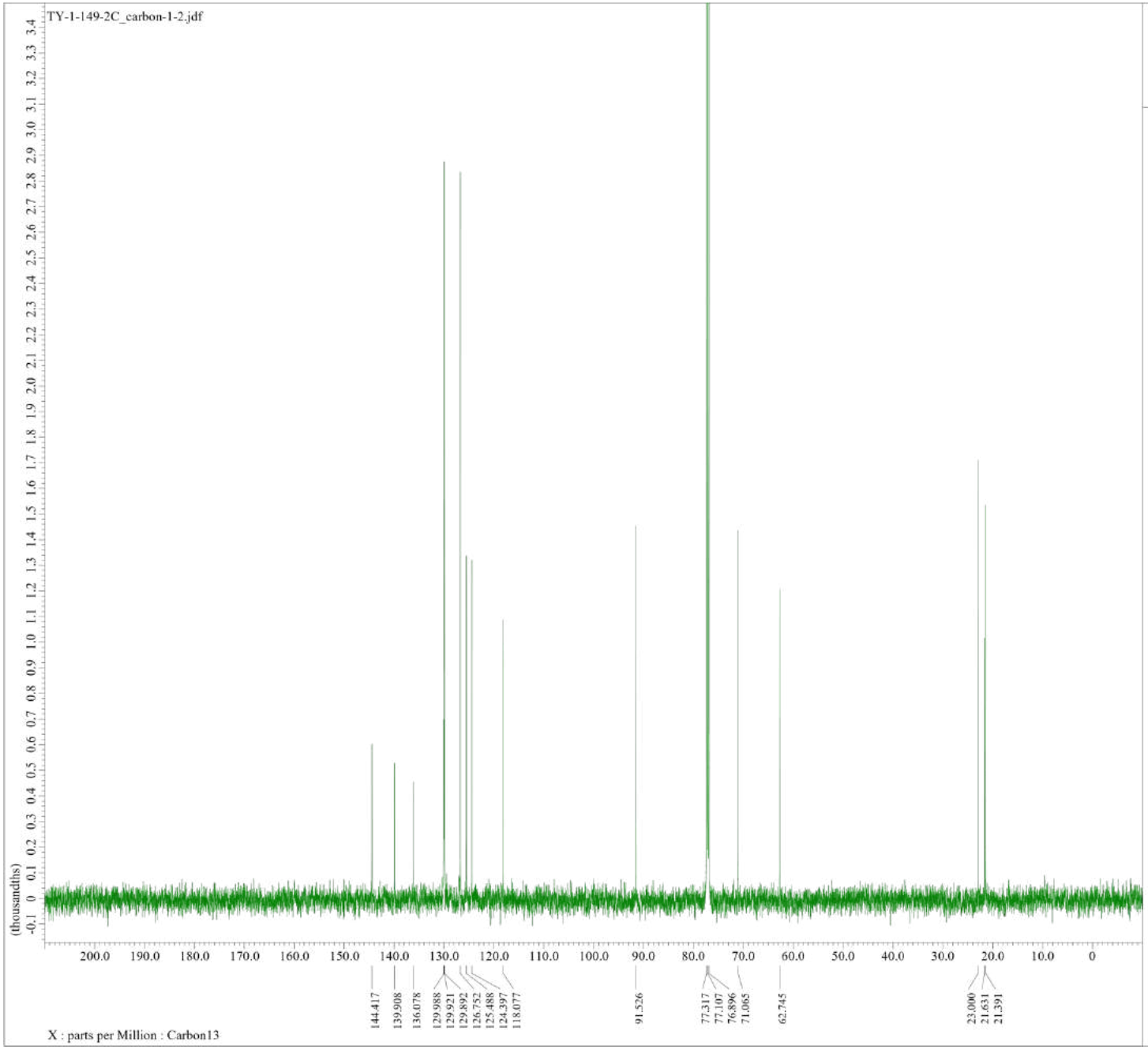
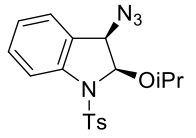


JEOL

Filename	= TY-1-149-2C_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-1-149-2C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-JUN-2021 16:14:
Revision_Time	= 17-JUN-2021 15:44:
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 207
Total_Scans	= 207
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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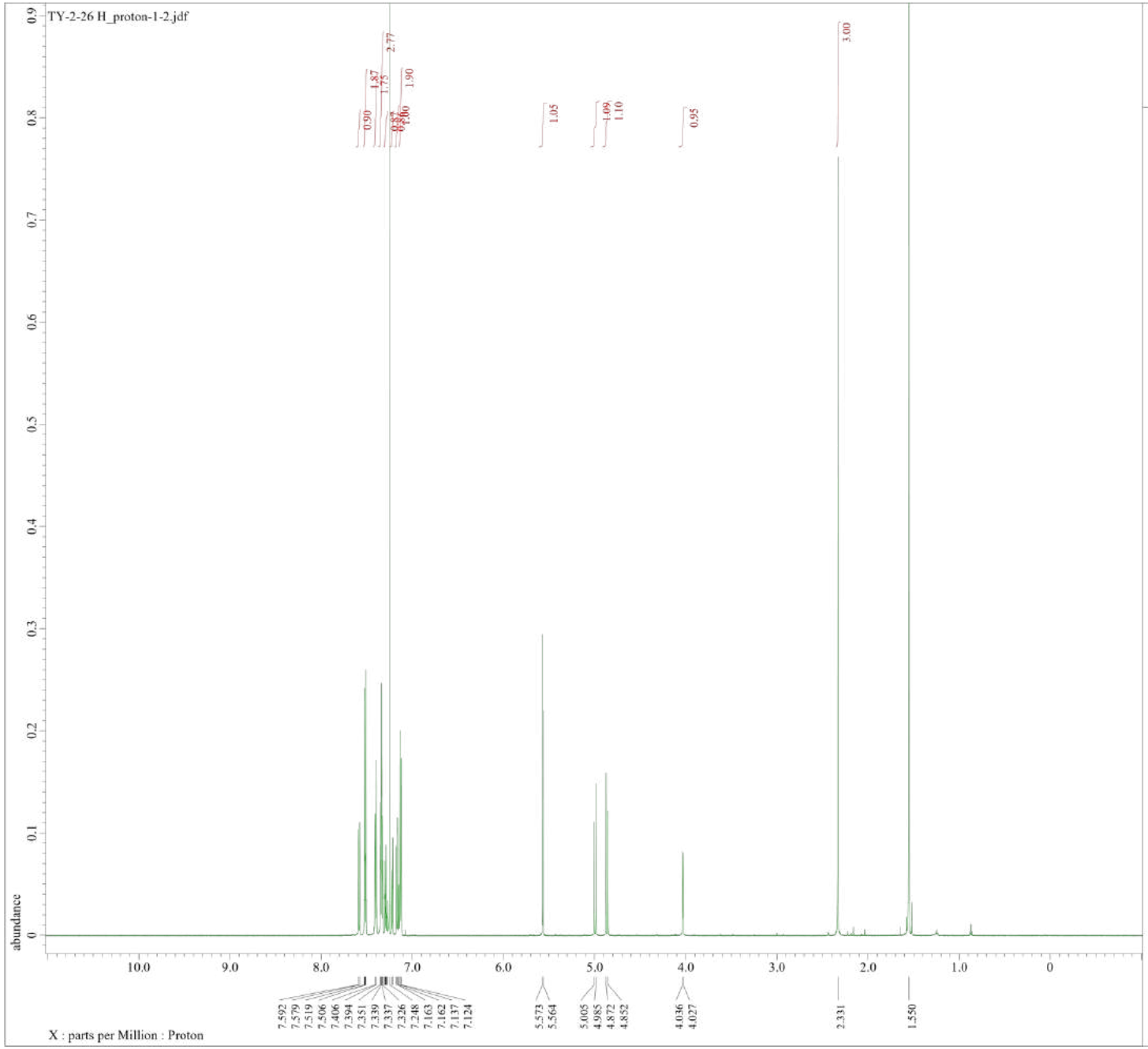
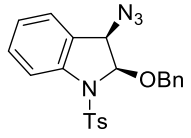


JEOL

Filename	= TY-2-26 H_proton-1-2.
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-26 H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-JUN-2021 15:52:10
Revision_Time	= 28-JUN-2021 15:52:09
Comment	= 2-OBn A&
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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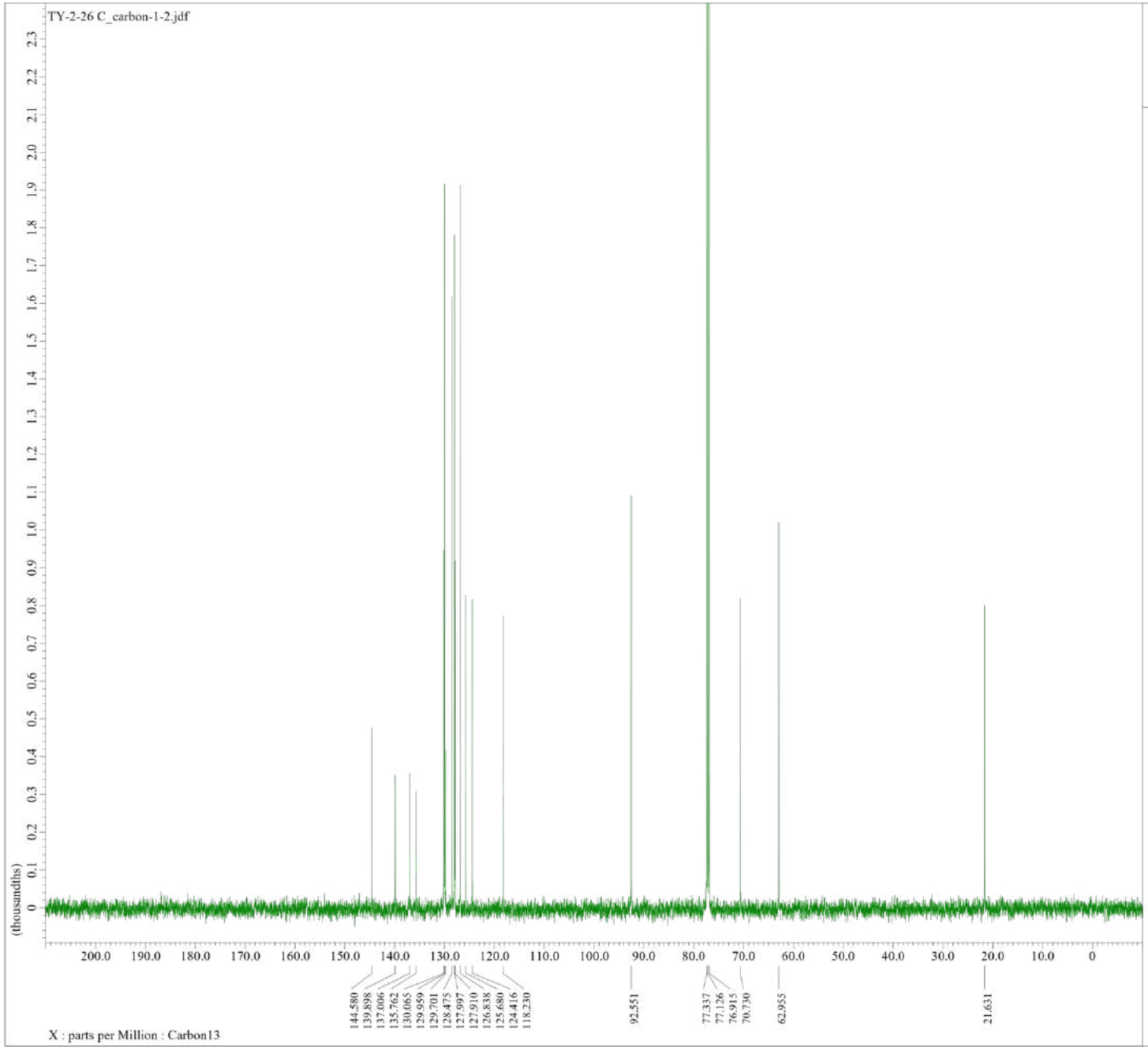
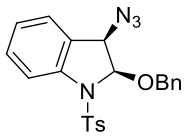


JEOL

Filename	= TY-2-26 C_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-26 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-JUN-2021 15:57:
Revision_Time	= 28-JUN-2021 16:00:
Comment	= 2-OBn AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 129
Total_Scans	= 129
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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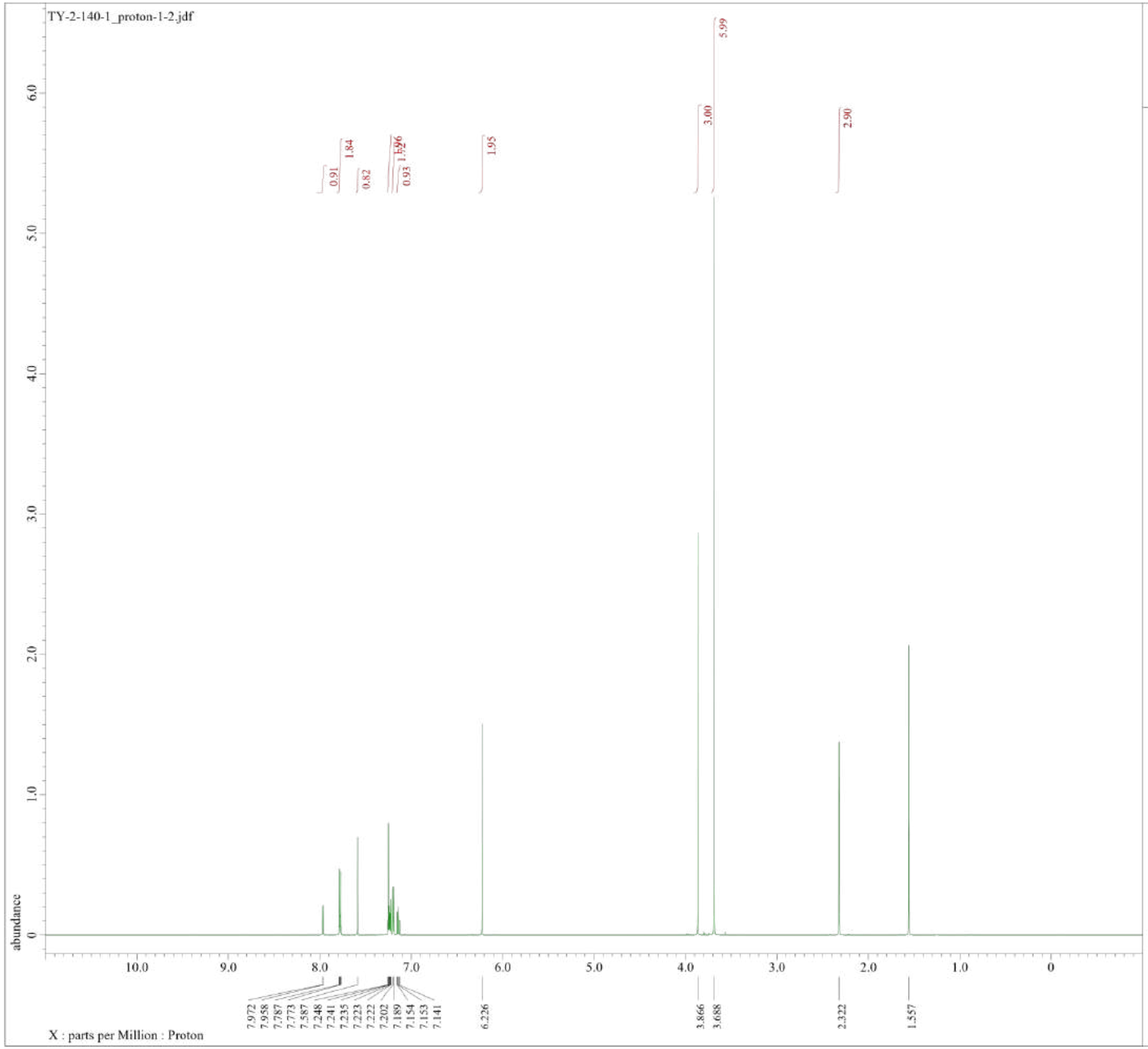
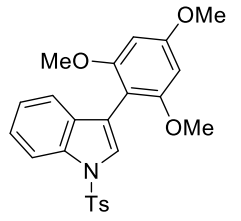


JEOL

Filename	= TY-2-140-1_proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-140-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-AUG-2021 21:39:30
Revision_Time	= 20-AUG-2021 21:58:02
Comment	= g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.9[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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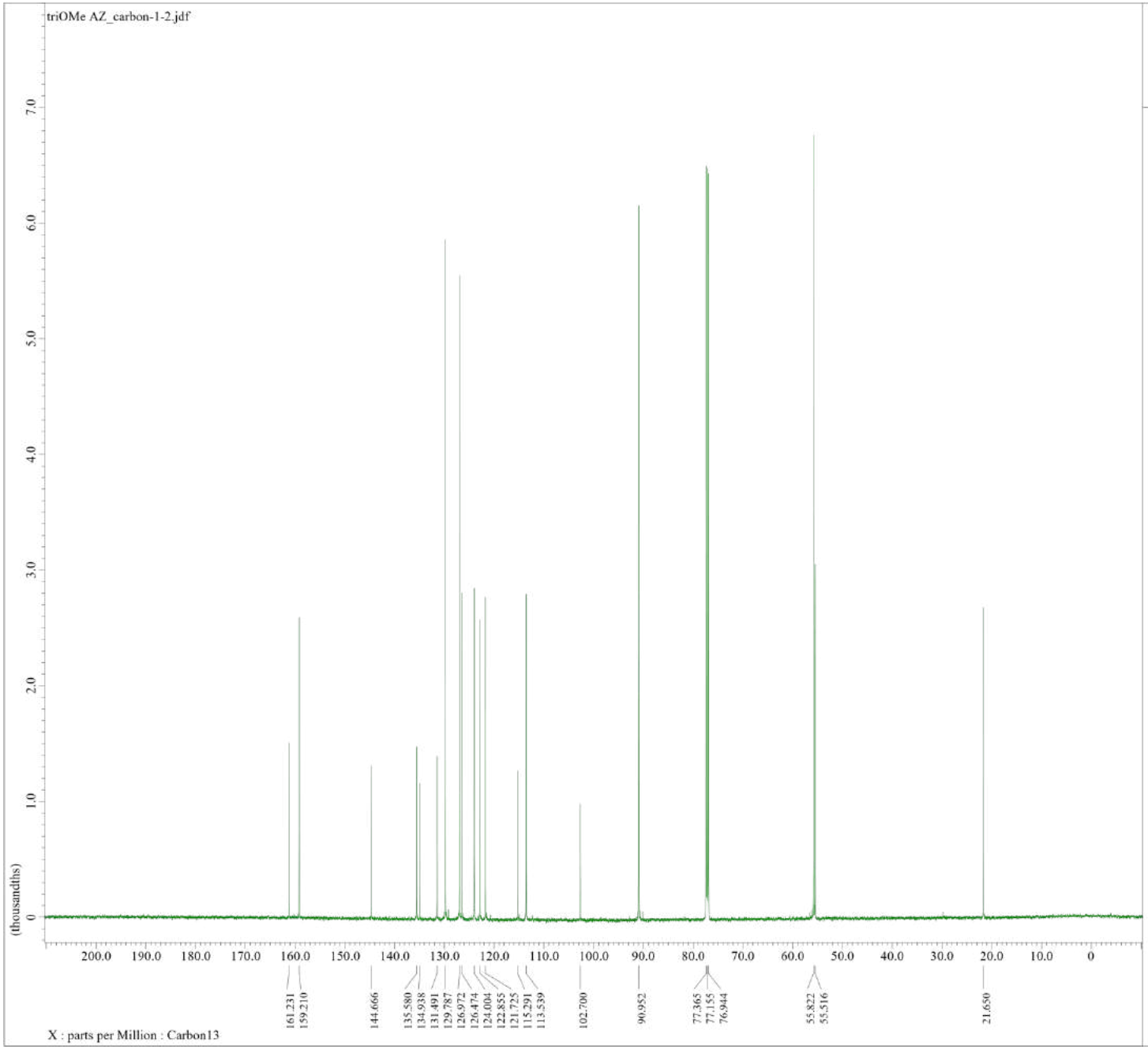
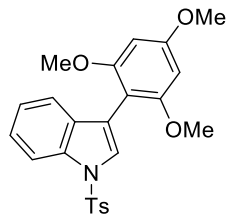


JEOL

Filename	= triOMe AZ_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= triOMe AZ
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-APR-2021 16:04:
Revision_Time	= 24-APR-2021 16:20:
Comment	= triOMe AZIN
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15[us]
Clipped	= FALSE
Scans	= 515
Total_Scans	= 515
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 19.9[dC]
X_90_Width	= 8.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 2.93333333[us]
Irr_Atn_Dec	= 26.162[dB]
Irr_Atn_Dec_Calc	= 26.162[dB]
Irr_Atn_Dec_Default_Calc	= 26.162[dB]
Irr_Atn_Noe	= 26.162[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



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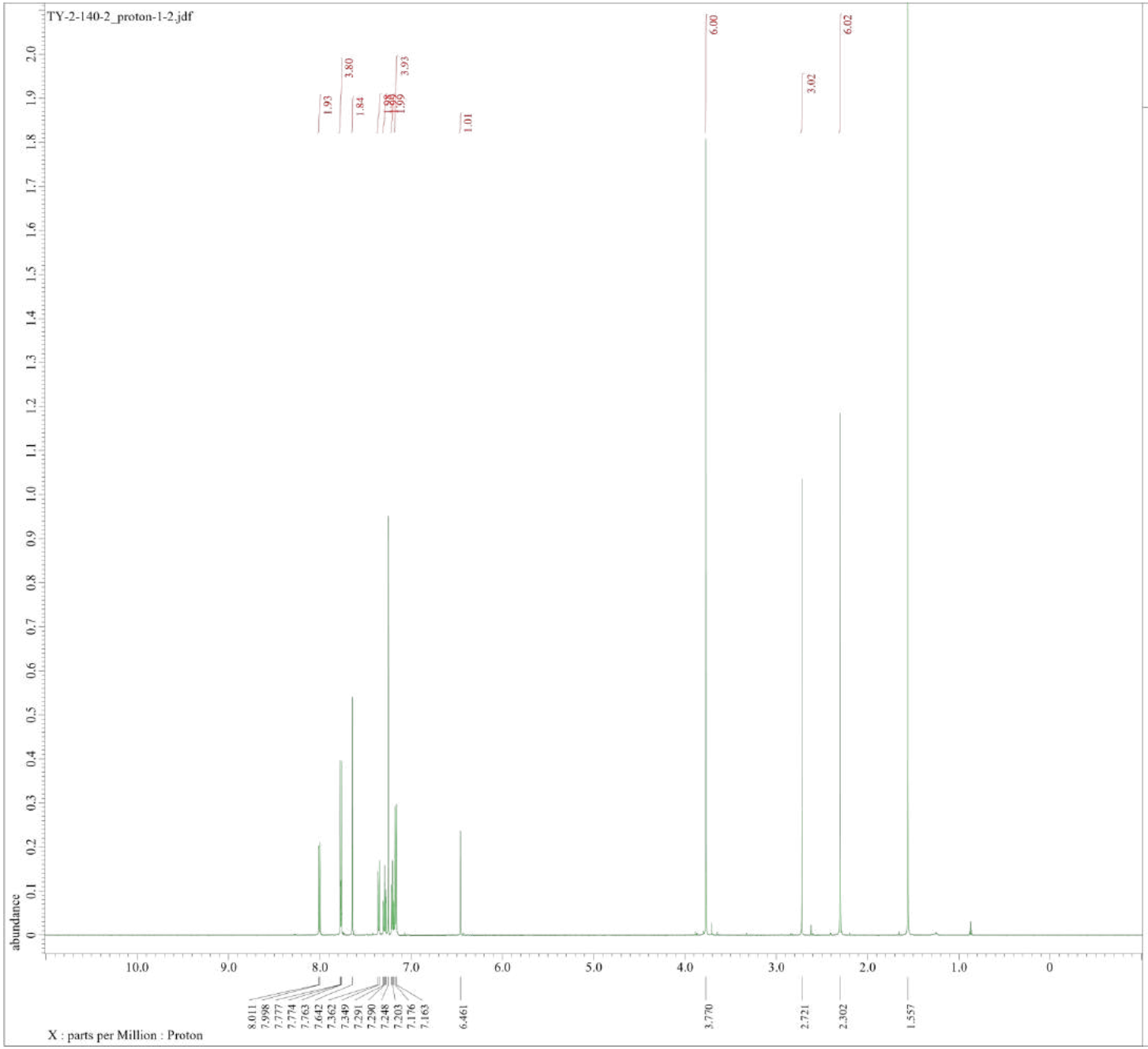


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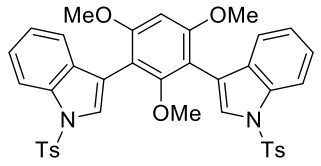
Filename              = TY-2-140-2_proton-1-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-140-2
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 20-AUG-2021 21:44:20
Revision_Time         = 20-AUG-2021 22:01:13

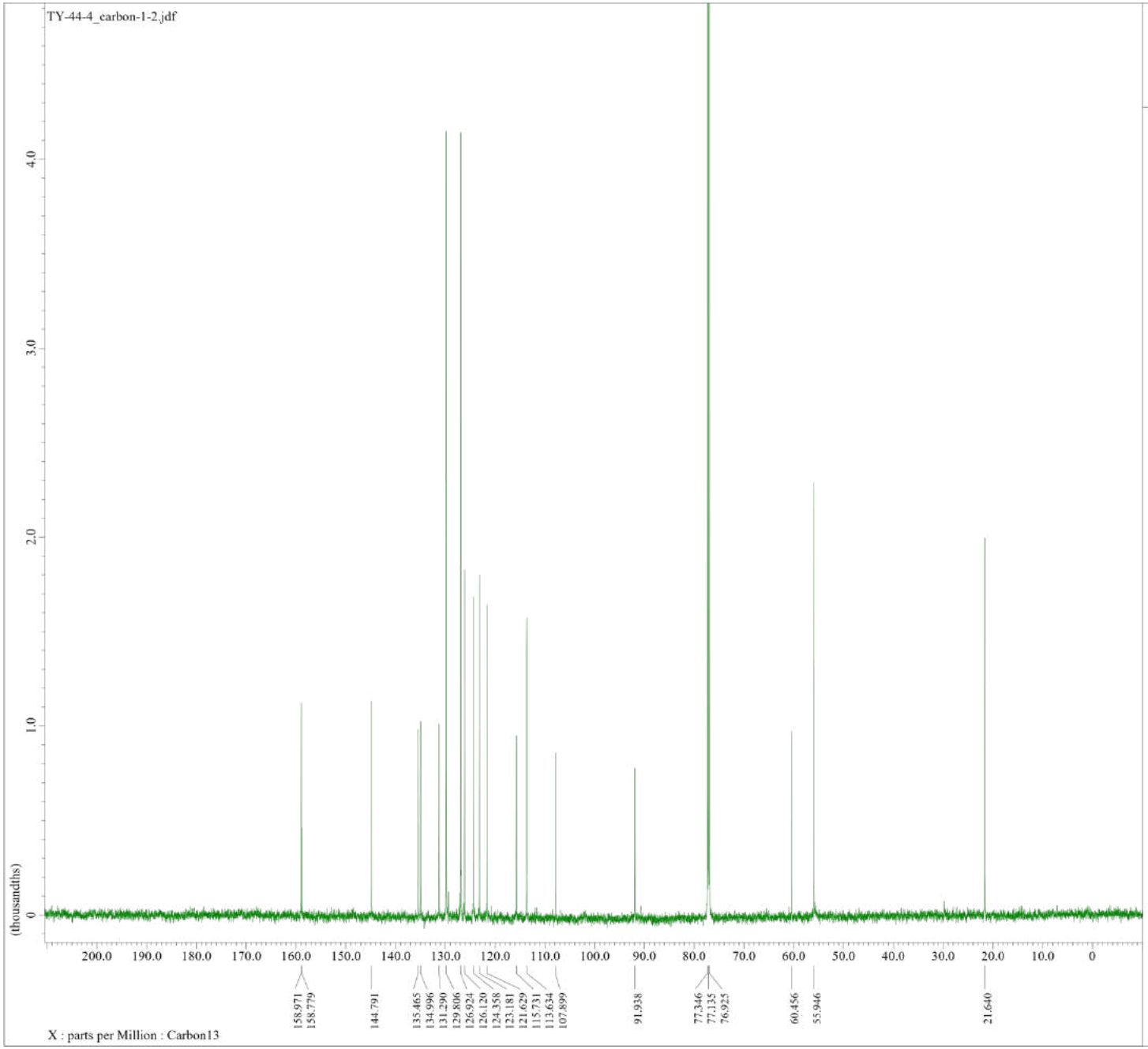
Comment               = g
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 20.9[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = (0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



6aa

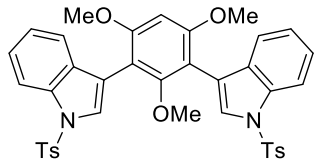



```
Filename                = TY-44-4_carbon-1-2
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = TY-44-4
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 11-MAY-2021 19:42:
Revision_Time           = 11-MAY-2021 19:55:

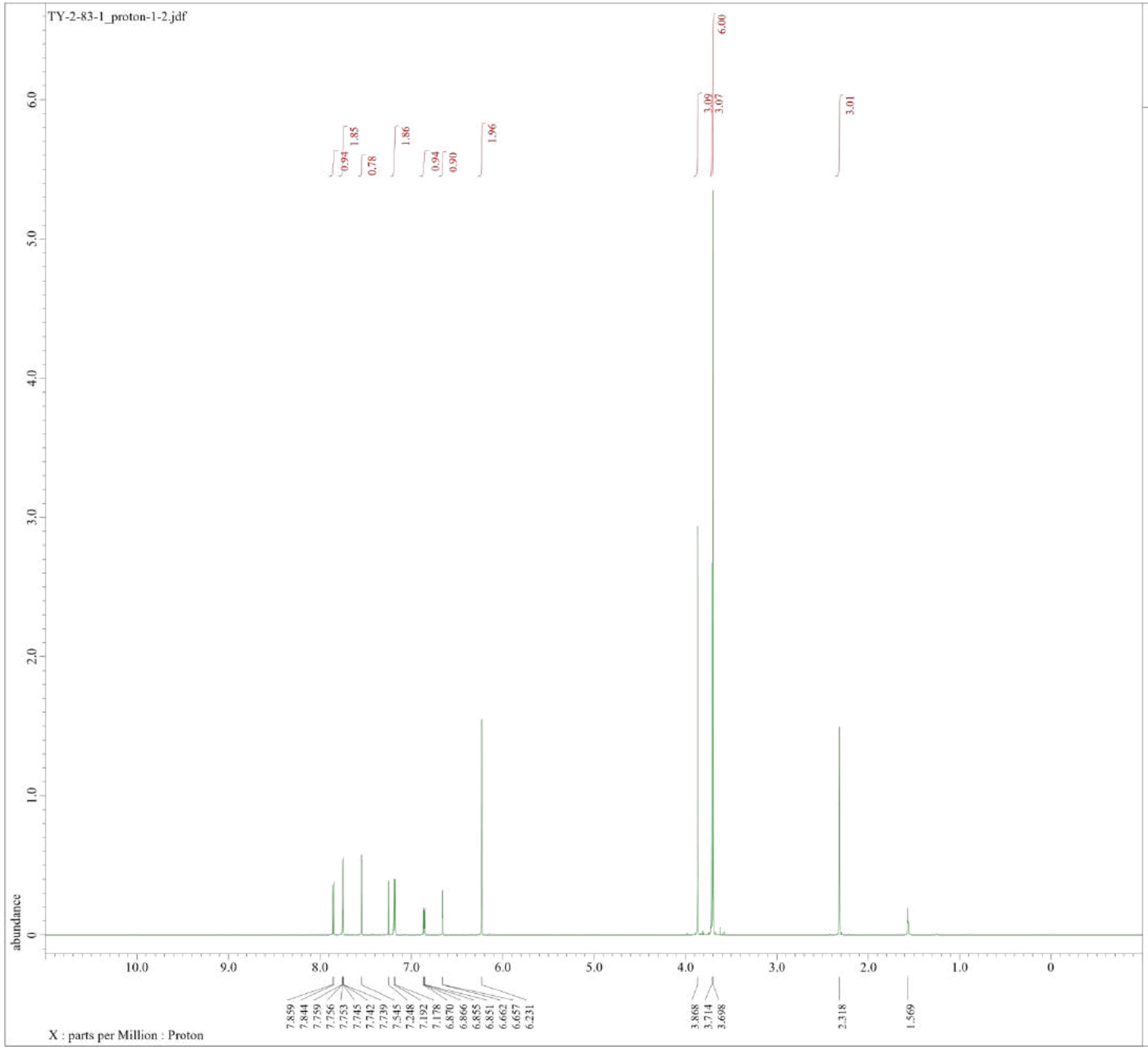
Comment                 = TY-44-4
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (60
X_Acq_Duration          = 0.69206016[s]
X_Domain                = Carbon13
X_Freq                  = 150.91343039[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 1.44496109[Hz]
X_Sweep                 = 47.34848485[kHz]
X_Sweep_Clipped         = 37.87878788[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 15[us]
Clipped                 = TRUE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 1[s]
Recvr_Gain              = 36
Temp_Get                = 20.1[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 0.69206016[s]
X_Angle                 = 30[deg]
X_Atn                   = 11[dB]
X_Pulse                 = 2.93333333[us]
Irr_Atn_Dec             = 26.162[dB]
Irr_Atn_Dec_Calc        = 26.162[dB]
Irr_Atn_Dec_Default_Calc = 26.162[dB]
Irr_Atn_Noe             = 26.162[dB]
Irr_Dec_Bandwidth_Hz    = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm   = 12.05794078[ppm]
Irr_Dec_Freq            = 600.1723046[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 76[us]
Irr_Pwidth_Default      = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1        = 76[us]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
Experiment_Path         = c:\Program Files\J
Initial_Wait            = 1[s]
Noe_Time                = 1[s]
Noe_Time_Flag           = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 1[s]
Repetition_Time         = 1.69206016[s]
```



6aa



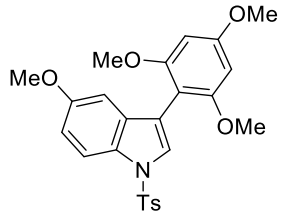
JEOL

```
Filename              = TY-2-83-1_proton-1-2.
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-83-1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 19-JUL-2021 10:32:37
Revision_Time         = 20-JUL-2021 14:13:59

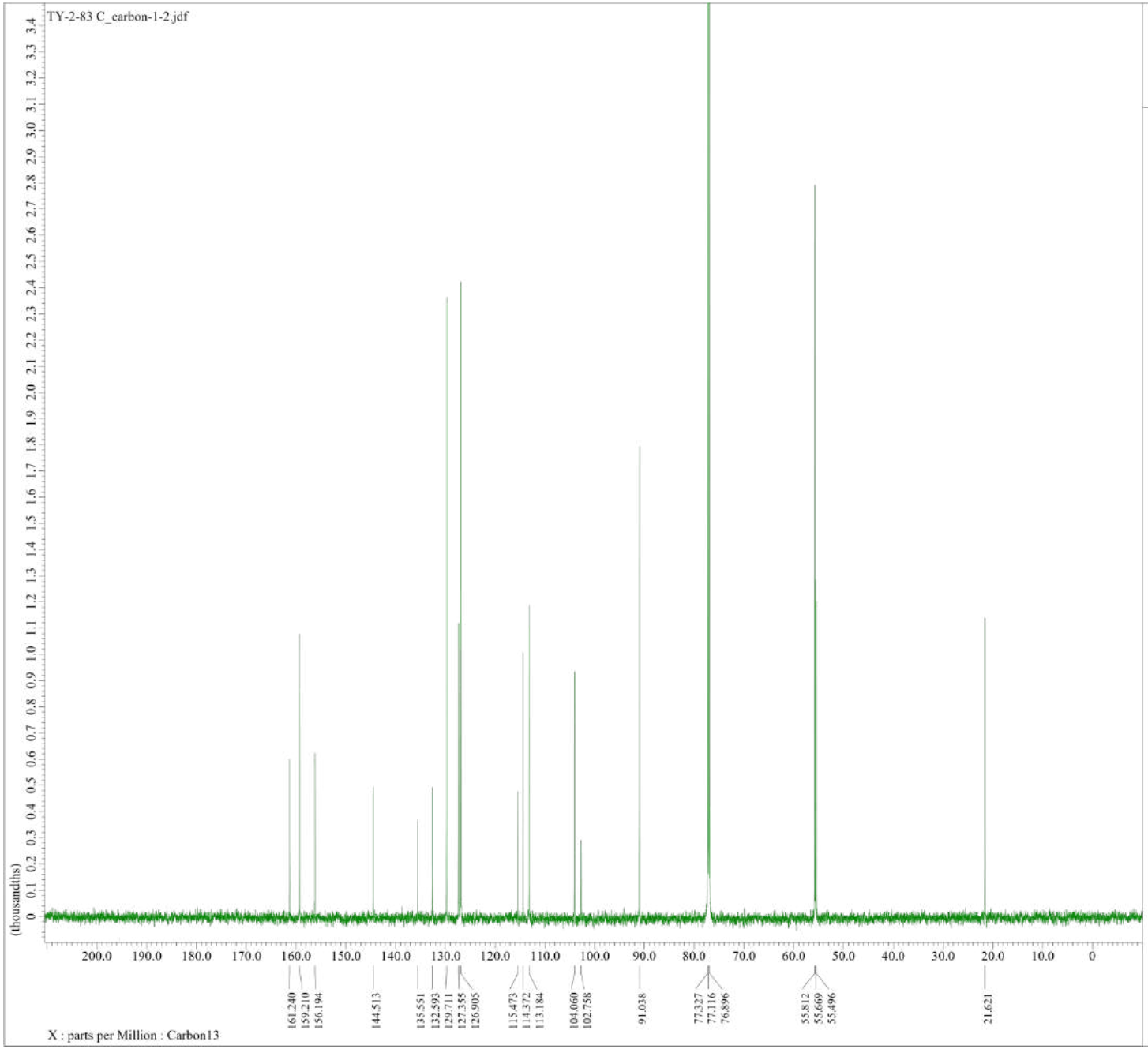
Comment               = 5-OMe triOMe
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 46
Temp_Get              = 21[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = (0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

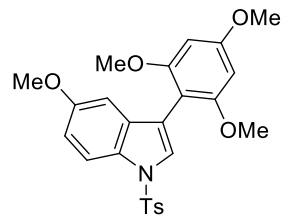


5ba

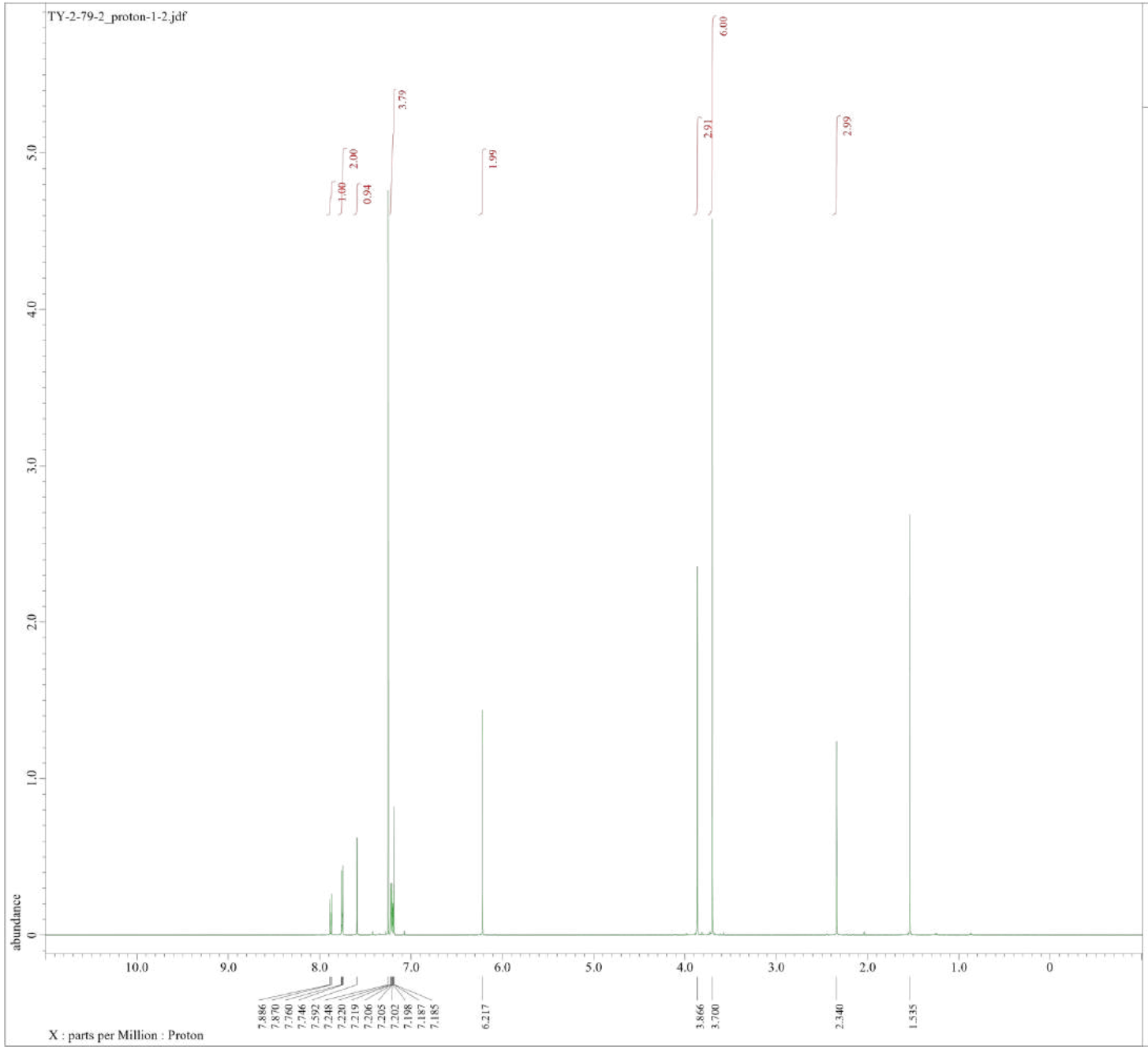


JEOL

Filename	= TY-2-83 C_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-83 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JUL-2021 13:11:
Revision_Time	= 20-JUL-2021 14:15:
Comment	= 5-OMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21.5[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



5ba

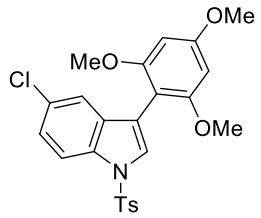



```
Filename              = TY-2-79-2_proton-1-2.
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-79-2
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 15-JUL-2021 18:55:03
Revision_Time         = 15-JUL-2021 19:25:58

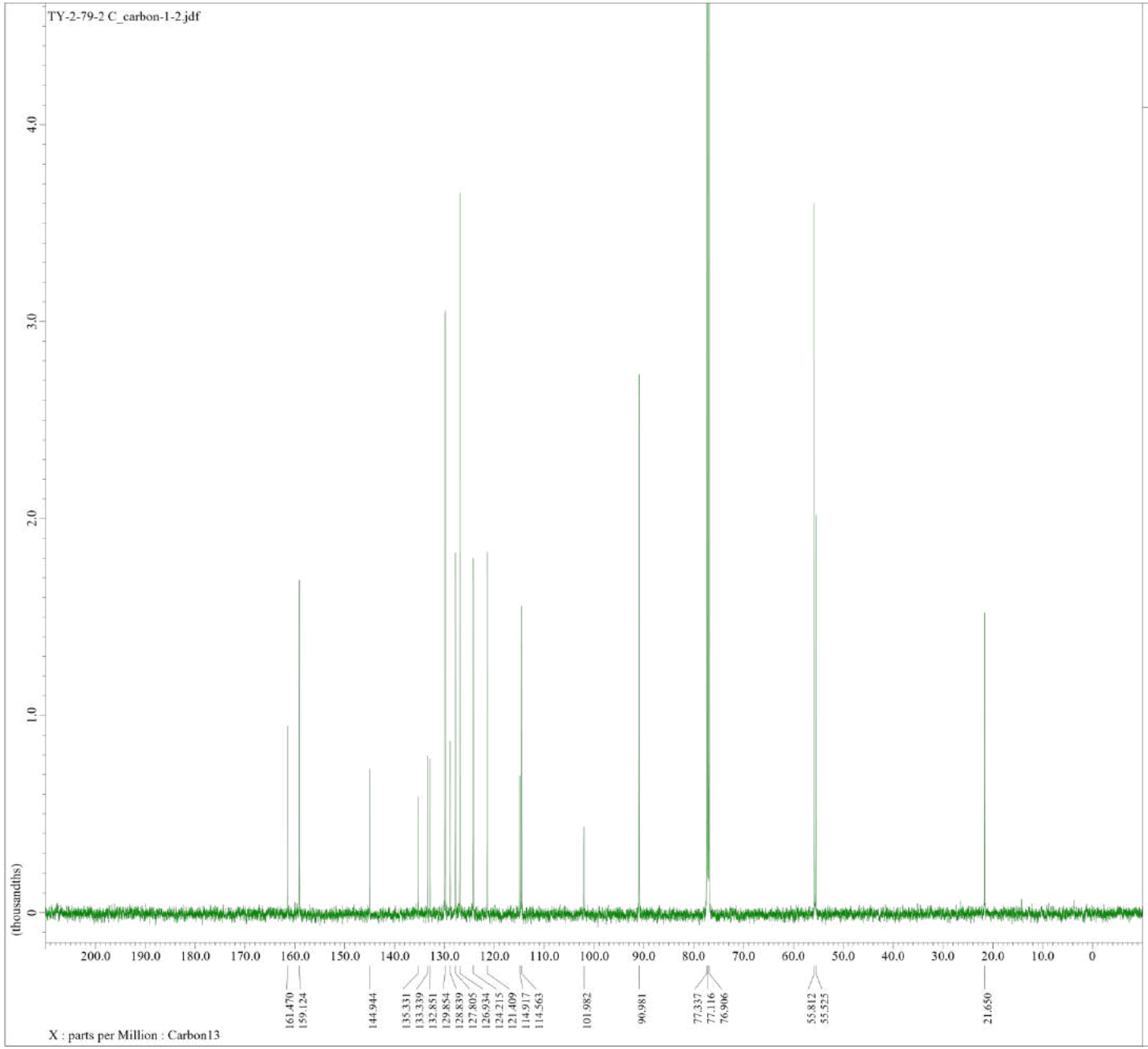
Comment               = 5Cl
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.90455552[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.34428676[Hz]
X_Sweep               = 11.28158845[kHz]
X_Sweep_Clipped       = 9.02527076[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 20.7[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.90455552[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = (0, 90, 270, 180, 180
Presat_Time           = 5[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time       = 7.90455552[s]
```

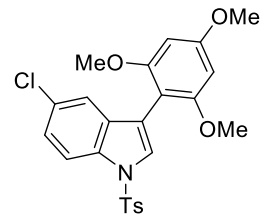


5ca

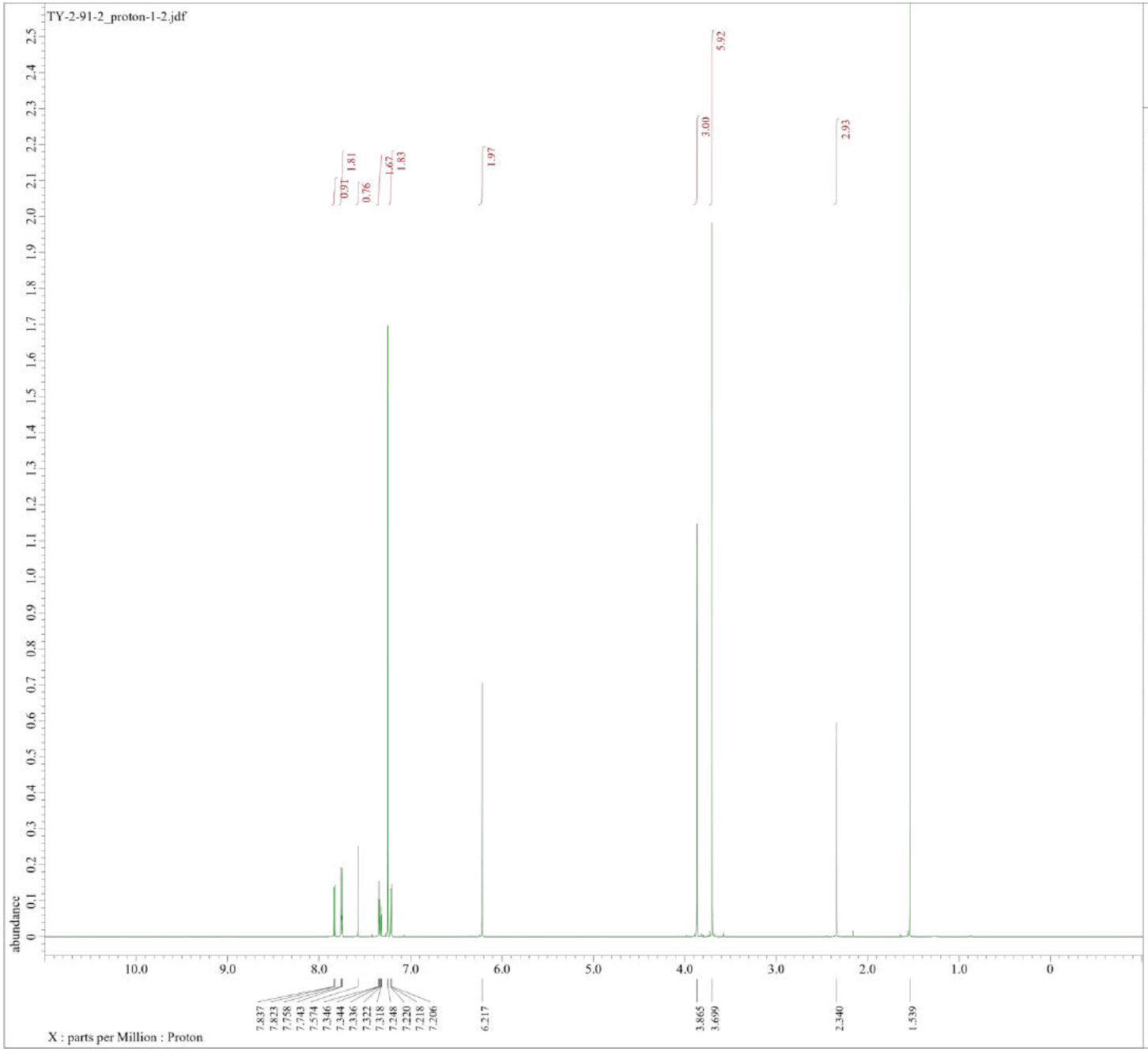


JEOL

Filename	= TY-2-79-2 C_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-79-2 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-JUL-2021 11:38:
Revision_Time	= 16-JUL-2021 11:58:
Comment	= 5-Cl
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]

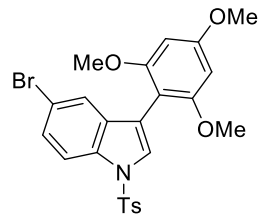


5ca

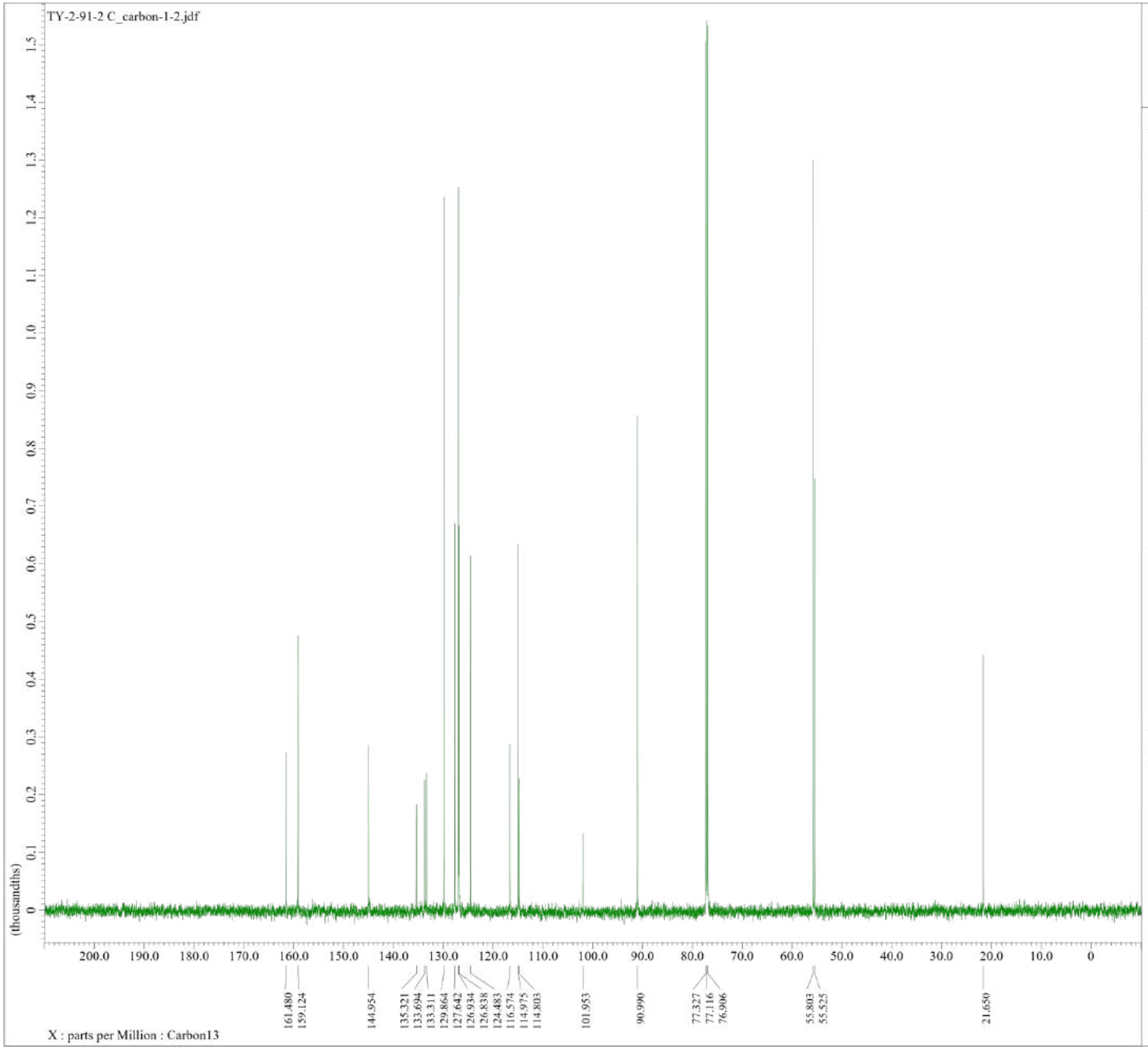


JEOL

Filename	= TY-2-91-2_proton-1-2.
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-91-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-AUG-2021 17:52:36
Revision_Time	= 4-AUG-2021 18:10:40
Comment	= 5-Br AZ triOMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21.2[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

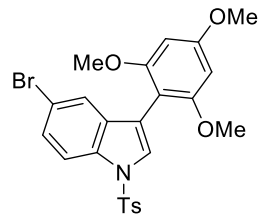


5da

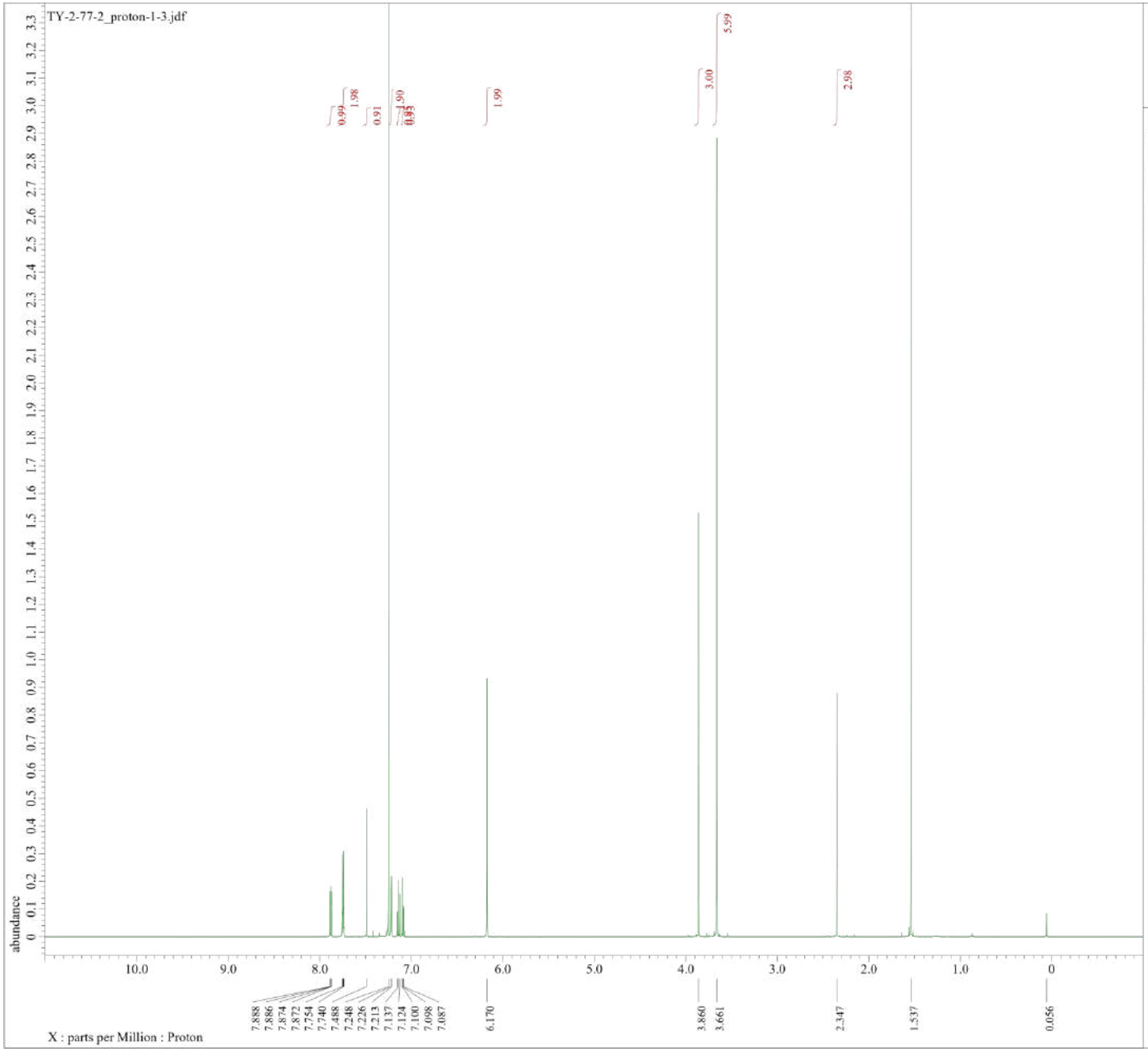


JEOL

Filename	= TY-2-91-2 C_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-91-2 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-AUG-2021 15:37:
Revision_Time	= 6-AUG-2021 15:52:
Comment	= 5-Br
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 515
Total_Scans	= 515
Relaxation_Delay	= 1[s]
Recvr_Gain	= 26
Temp_Get	= 21.8[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



5da

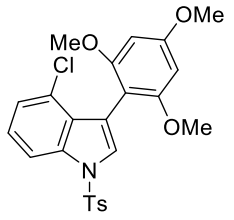



```
Filename              = TY-2-77-2_proton-1-3.
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-77-2
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 15-JUL-2021 18:37:17
Revision_Time         = 15-JUL-2021 19:23:15

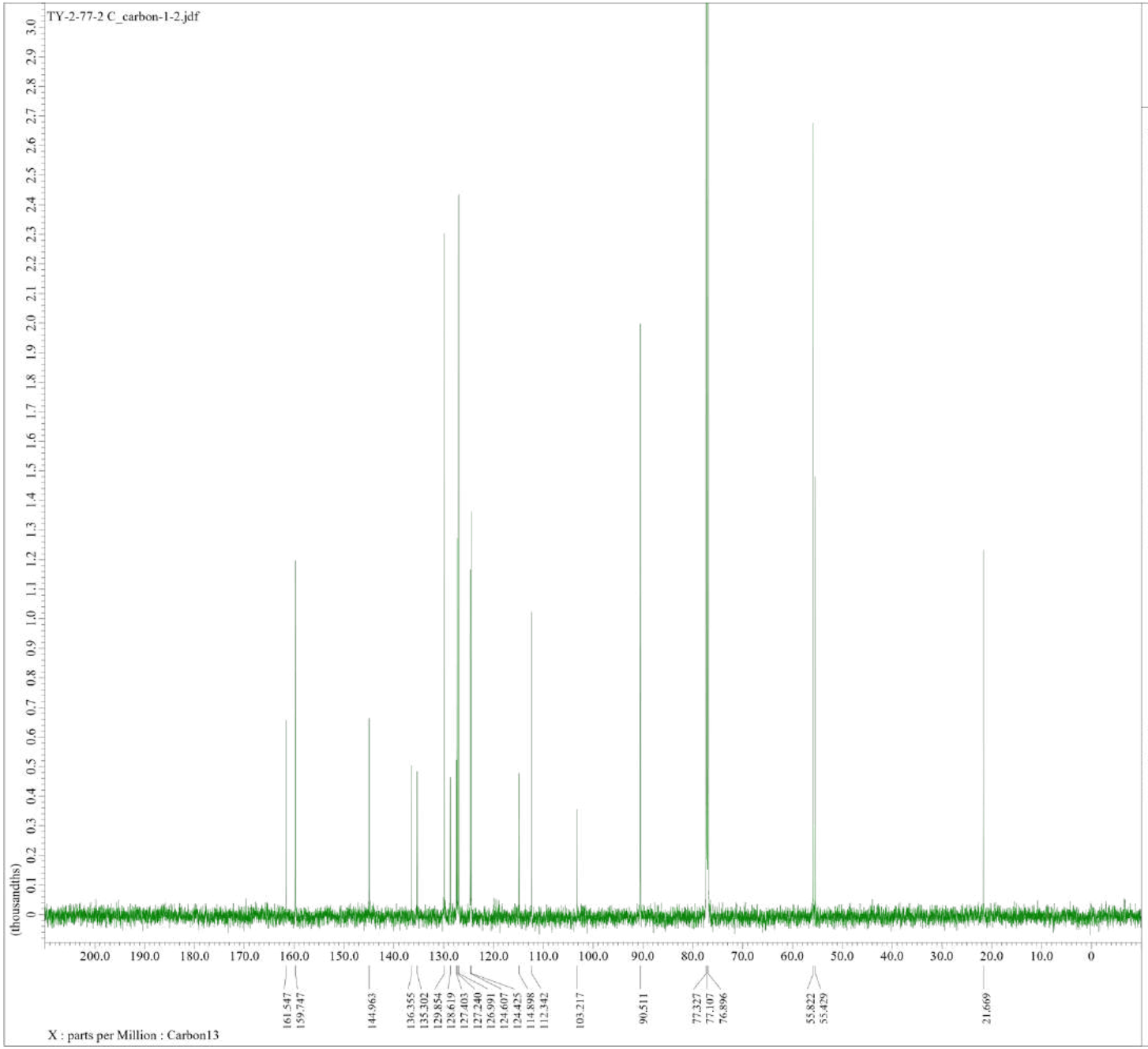
Comment               = 4Cl
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.90455552[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.34428676[Hz]
X_Sweep               = 11.28158845[kHz]
X_Sweep_Clipped       = 9.02527076[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 20.8[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.90455552[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = (0, 90, 270, 180, 180
Presat_Time           = 5[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time       = 7.90455552[s]
```

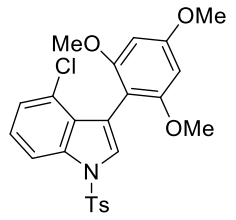


5ea

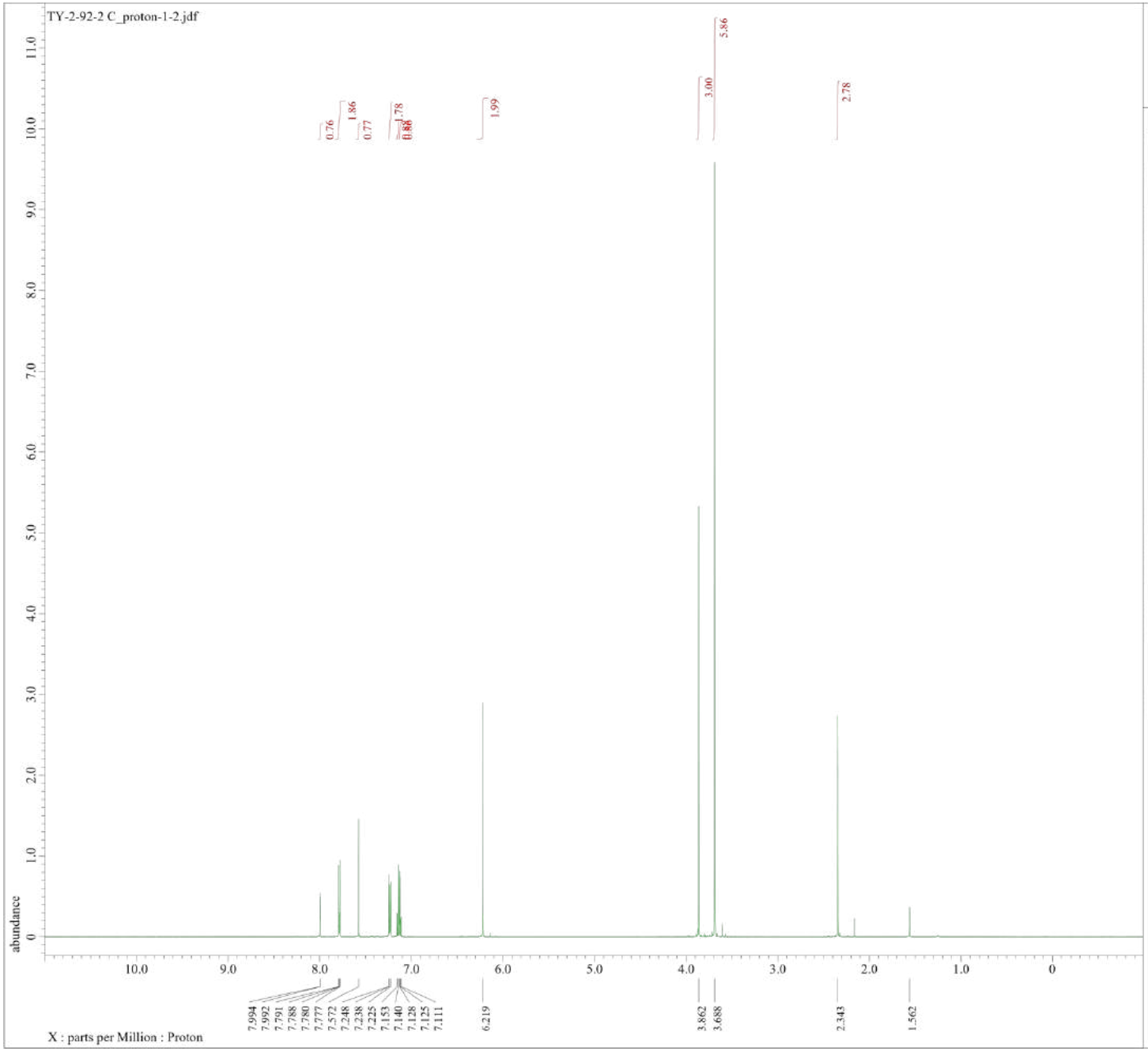


JEOL

Filename	= TY-2-77-2 C_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-77-2 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-JUL-2021 11:09:
Revision_Time	= 16-JUL-2021 11:29:
Comment	= 4-Cl
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]

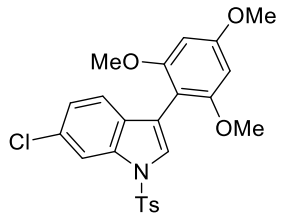


5ea



JEOL

Filename	= TY-2-92-2 C_proton-1-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-92-2 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-JUL-2021 19:34:44
Revision_Time	= 24-JUL-2021 19:35:01
Comment	= 6-ClAZ fr2
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 46
Temp_Get	= 21.2[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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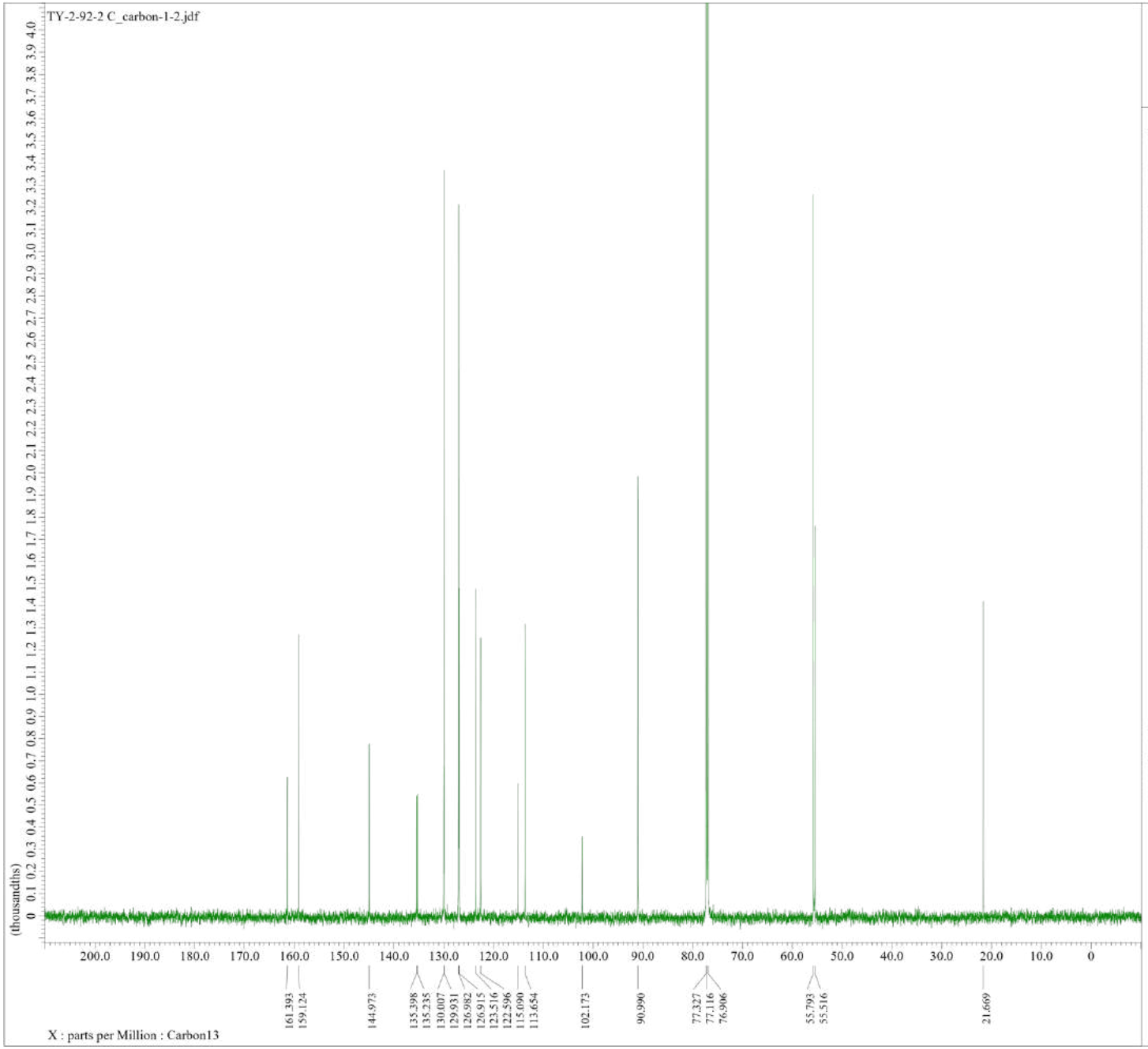
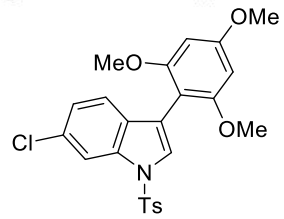


JEOL

Filename	= TY-2-92-2 C_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-92-2 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-JUL-2021 18:18:
Revision_Time	= 24-JUL-2021 19:16:
Comment	= 6-ClAZ fr2
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 641
Total_Scans	= 641
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21.3[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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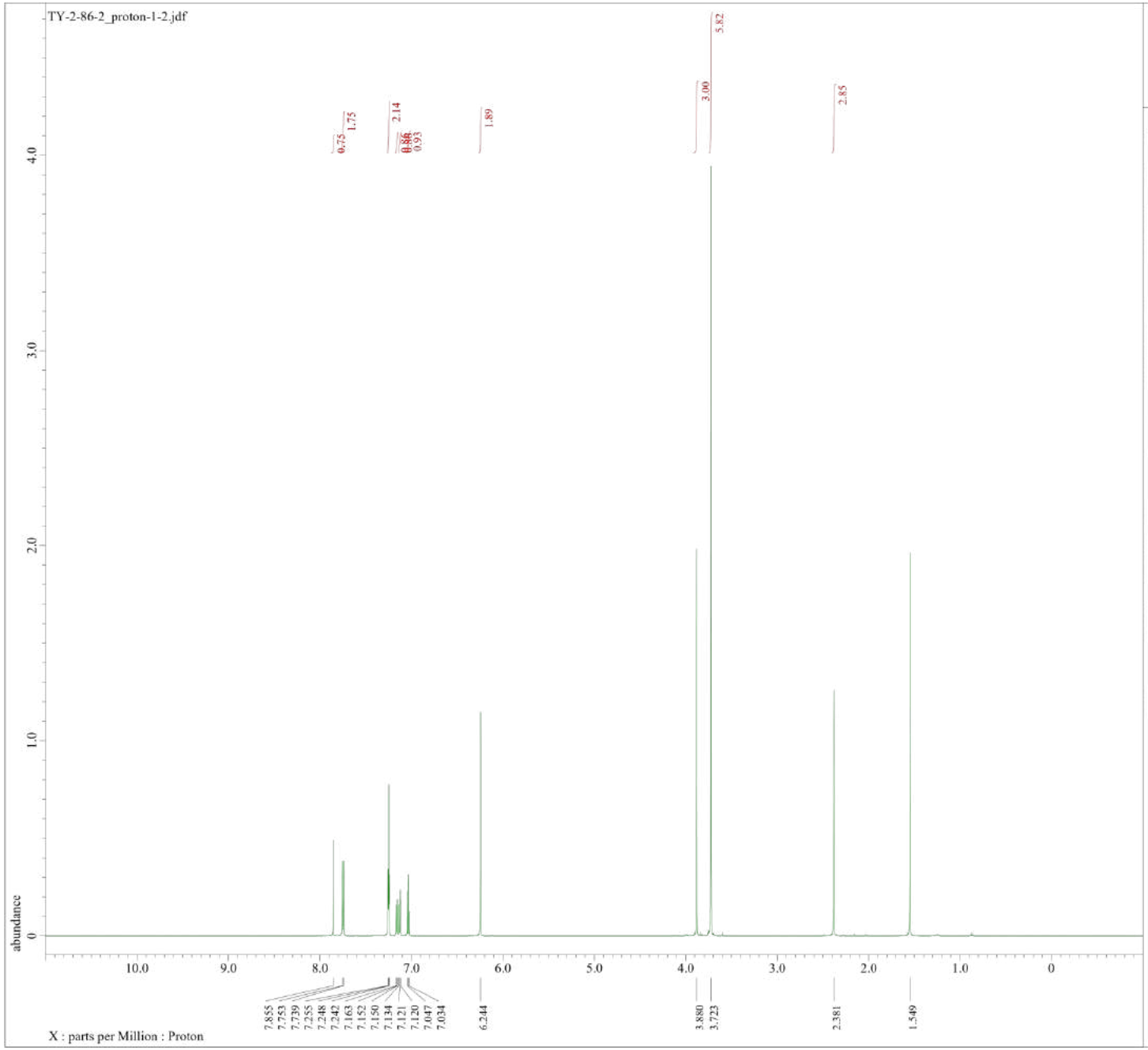


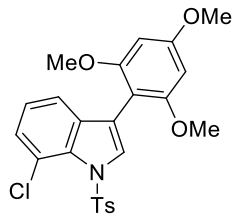
JEOL

```
Filename              = TY-2-86-2_proton-1-2.
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-86-2
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 16-AUG-2021 20:56:18
Revision_Time         = 16-AUG-2021 21:00:31

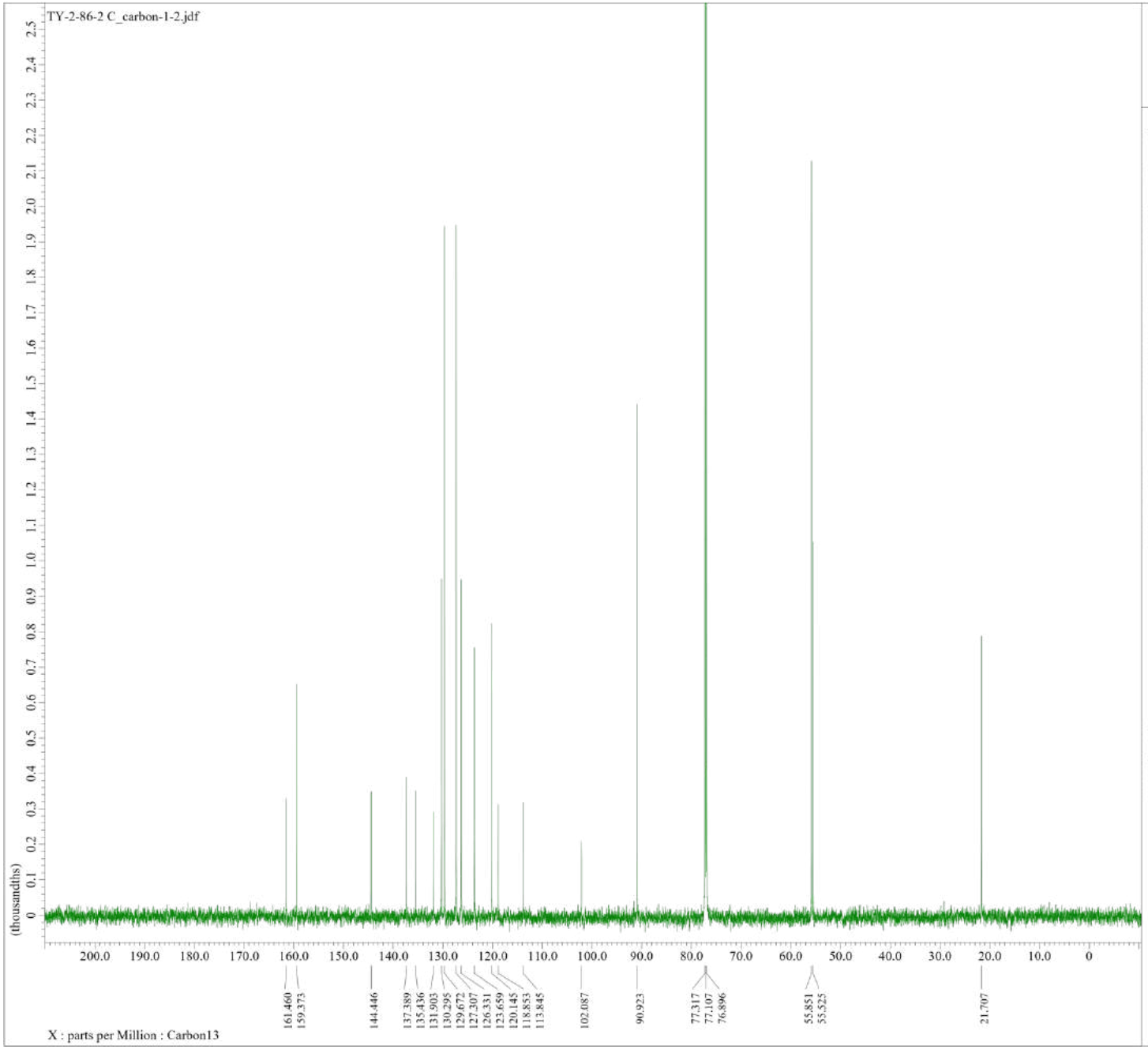
Comment               = 7-Cl A& fr2
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 21[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

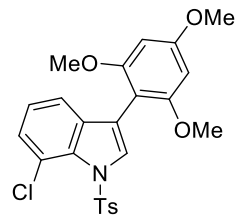


5ga

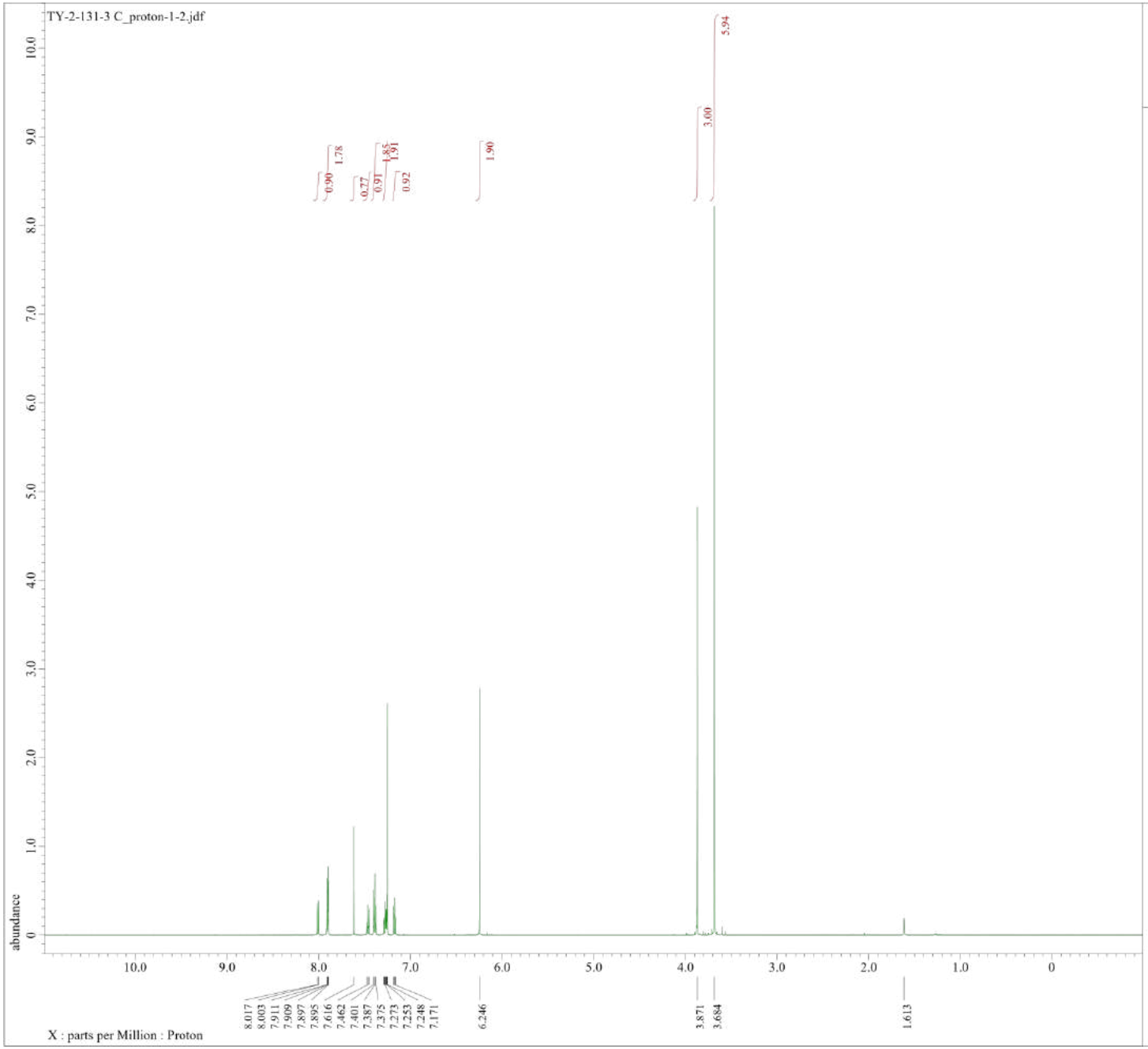


JEOL

Filename	= TY-2-86-2 C_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-86-2 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-AUG-2021 14:30:
Revision_Time	= 17-AUG-2021 15:03:
Comment	= 7-Cl AZ triOMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

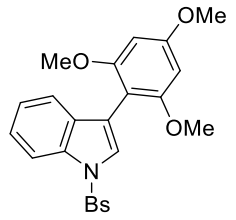


5ga

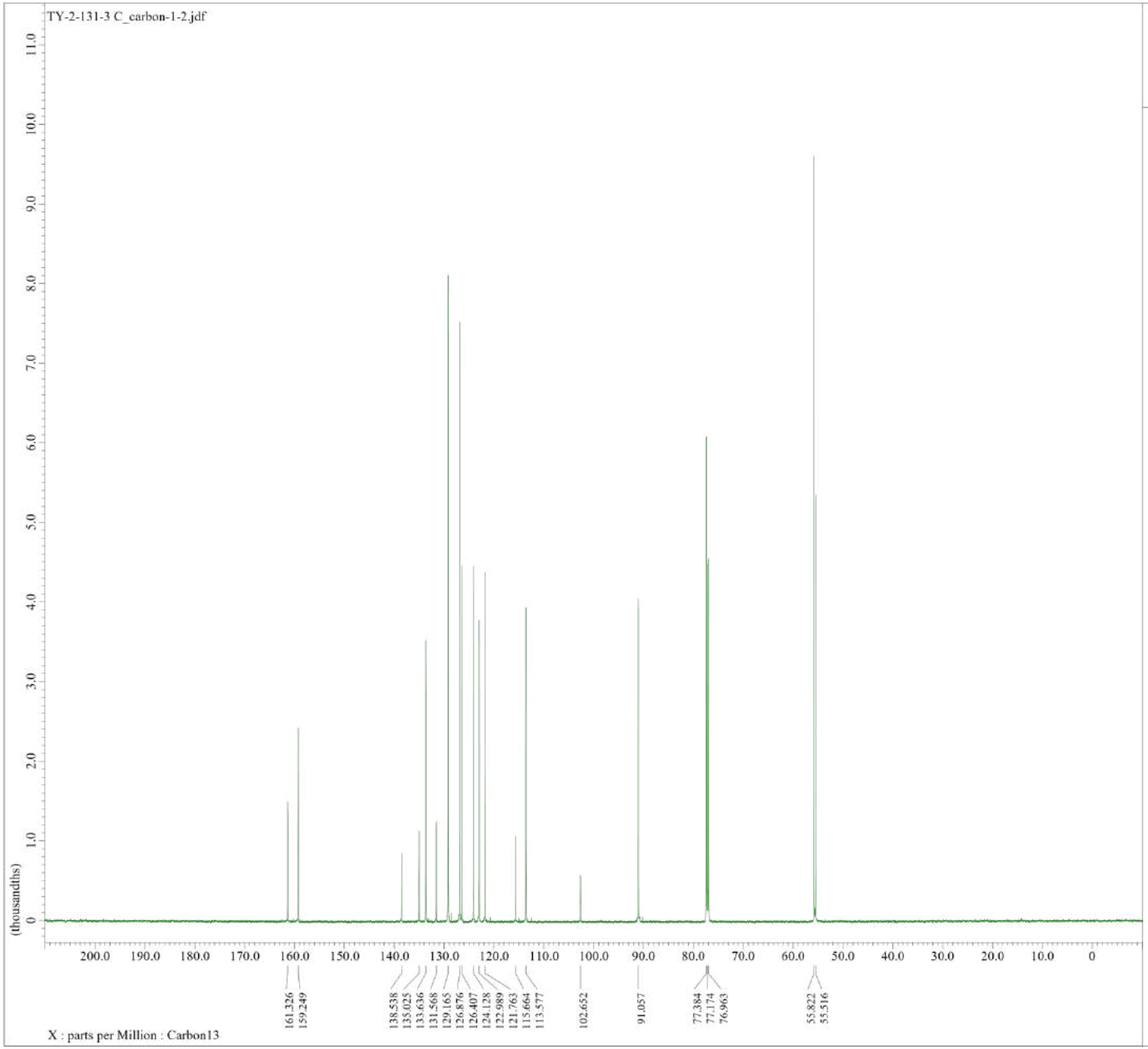


JEOL

Filename	= TY-2-131-3 C_proton-1
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-131-3 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-AUG-2021 21:22:27
Revision_Time	= 17-AUG-2021 21:25:38
Comment	= Bs AZ triOMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

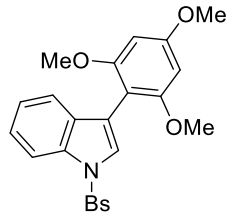


5ha

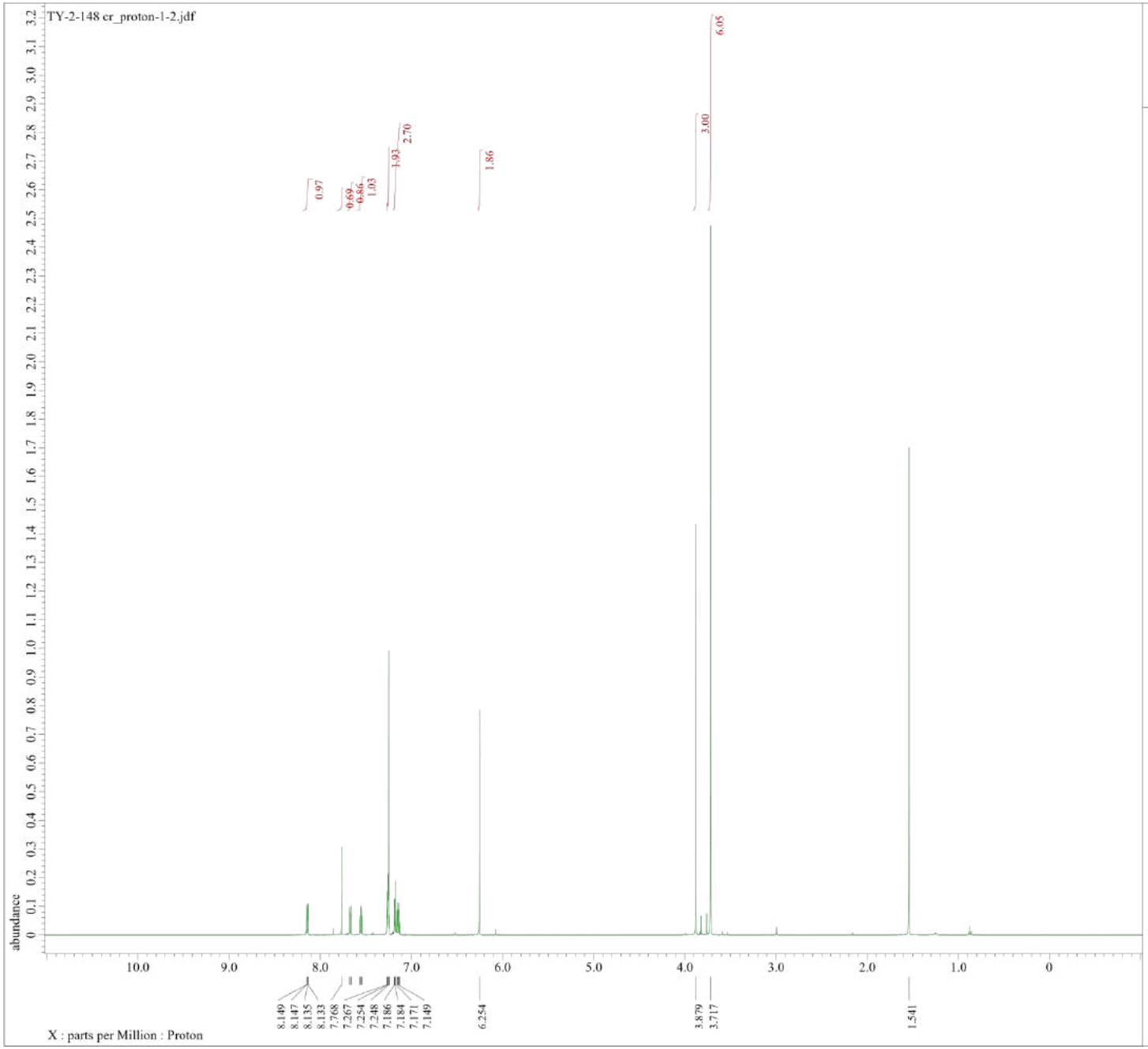


JEOL

Filename	= TY-2-131-3 C_carbo
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-131-3 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-AUG-2021 23:12:
Revision_Time	= 18-AUG-2021 08:43:
Comment	= Bs AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 4096
Total_Scans	= 4096
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



5ha



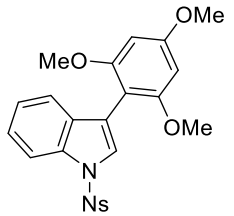
JEOL

```
Filename              = TY-2-148 cr_proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-148 cr
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 24-AUG-2021 22:48:08
Revision_Time         = 25-AUG-2021 08:34:15

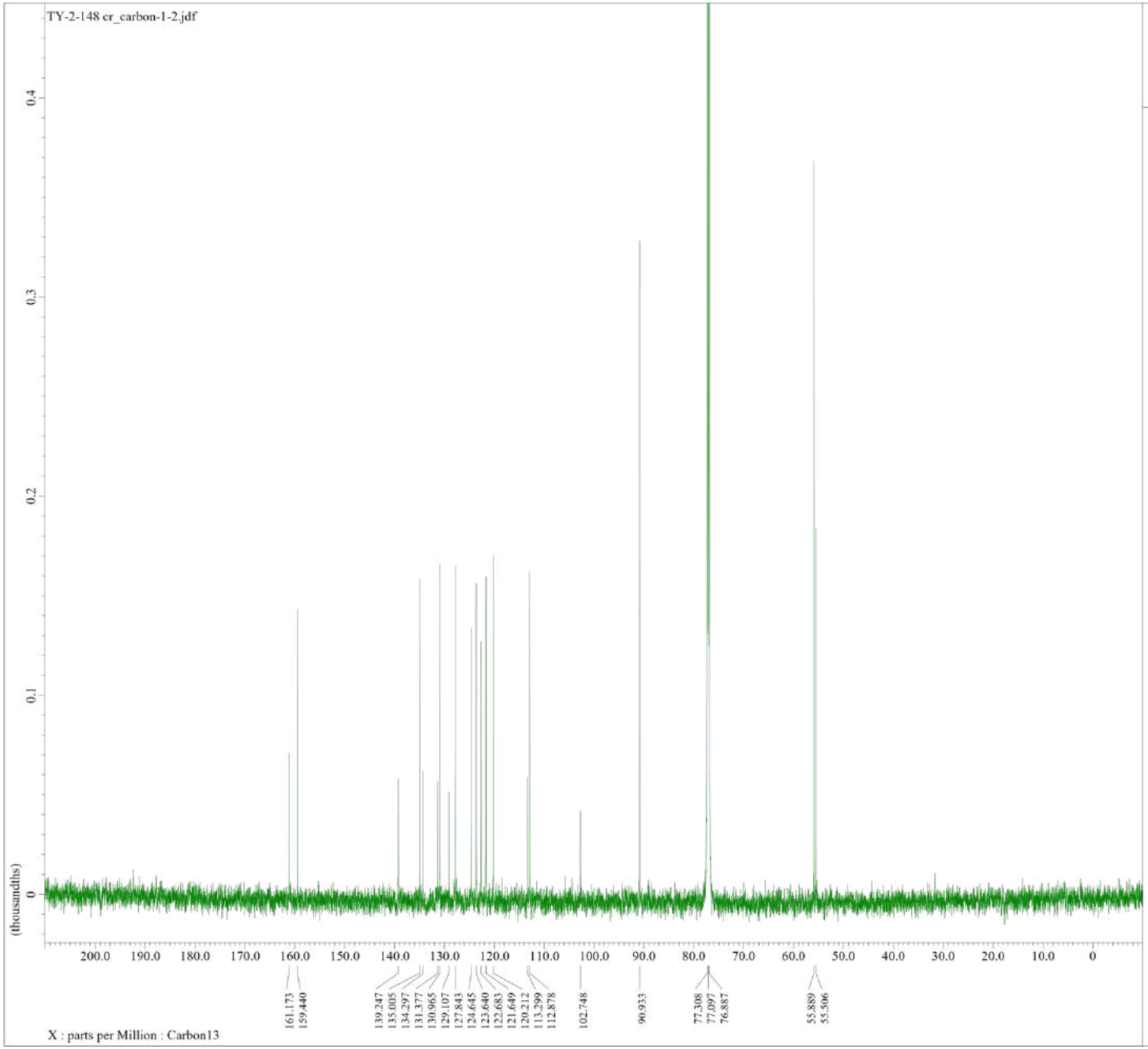
Comment               = Ns AE
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 21[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = (0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

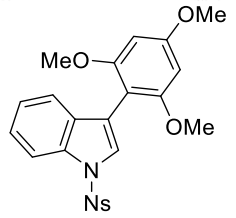


5ia

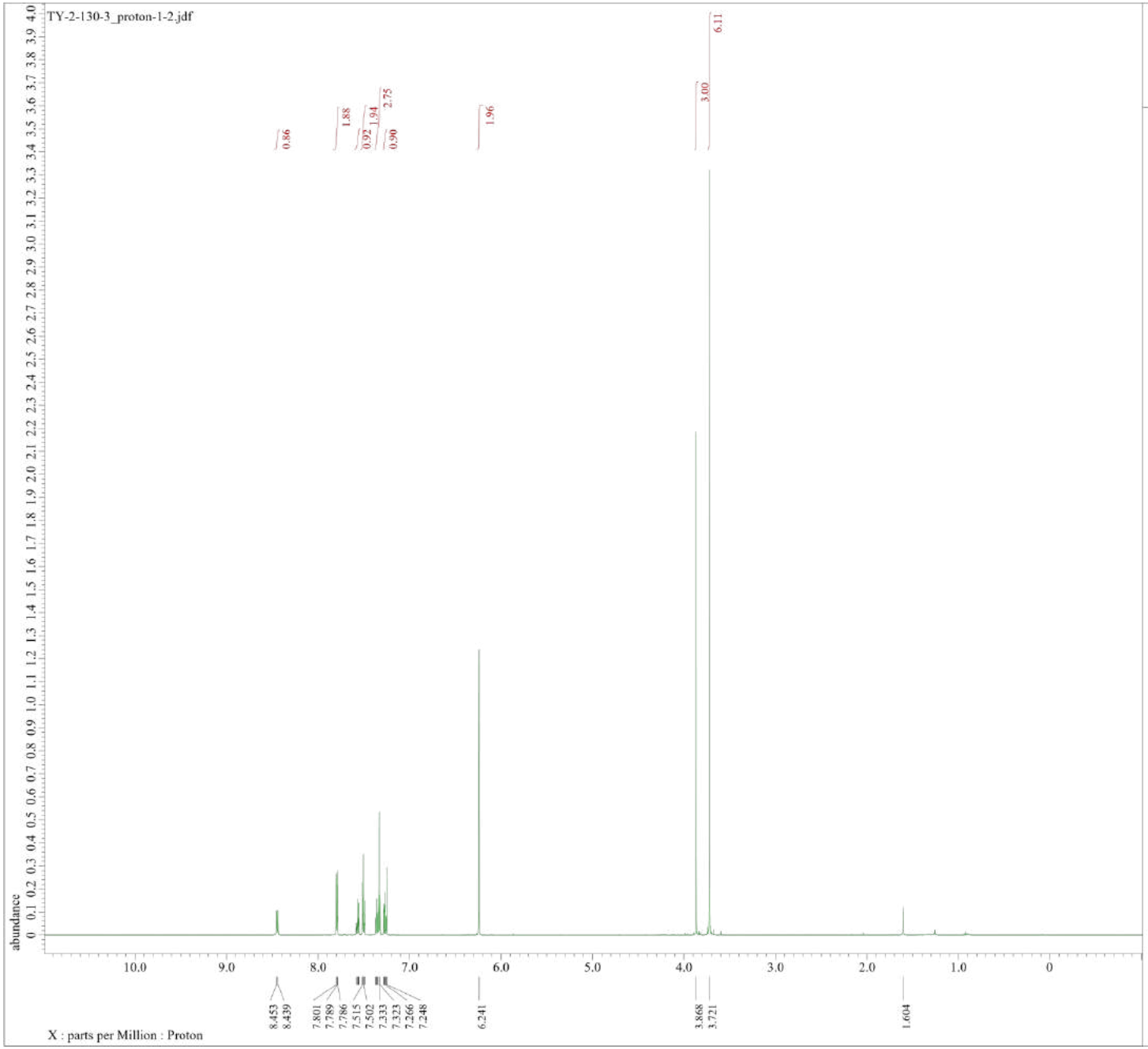


JEOL

Filename	= TY-2-148 cr_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-148 cr
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-AUG-2021 00:07:
Revision_Time	= 25-AUG-2021 08:36:
Comment	= Ns AE
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 15220
Total_Scans	= 15220
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



5ia



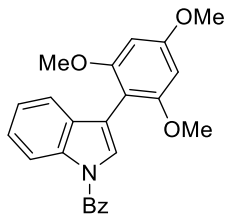
JEOL

```
Filename              = TY-2-130-3_proton-1-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-130-3
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 16-AUG-2021 20:33:09
Revision_Time         = 16-AUG-2021 20:35:07

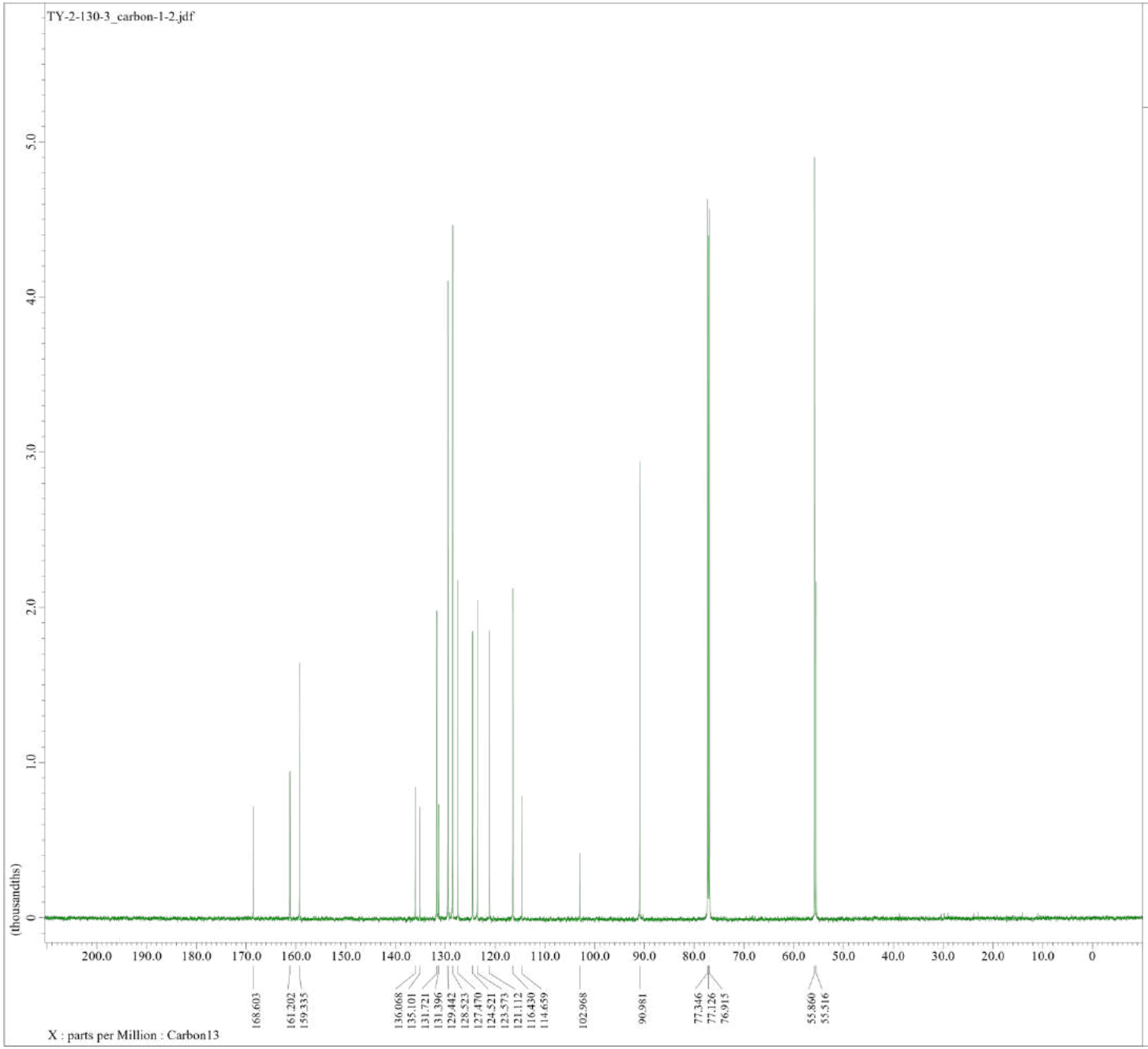
Comment               = Bz AE fr3
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

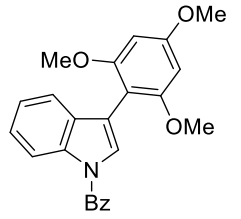
Relaxation_Delay      = 1[s]
Recvr_Gain            = 36
Temp_Get              = 21[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



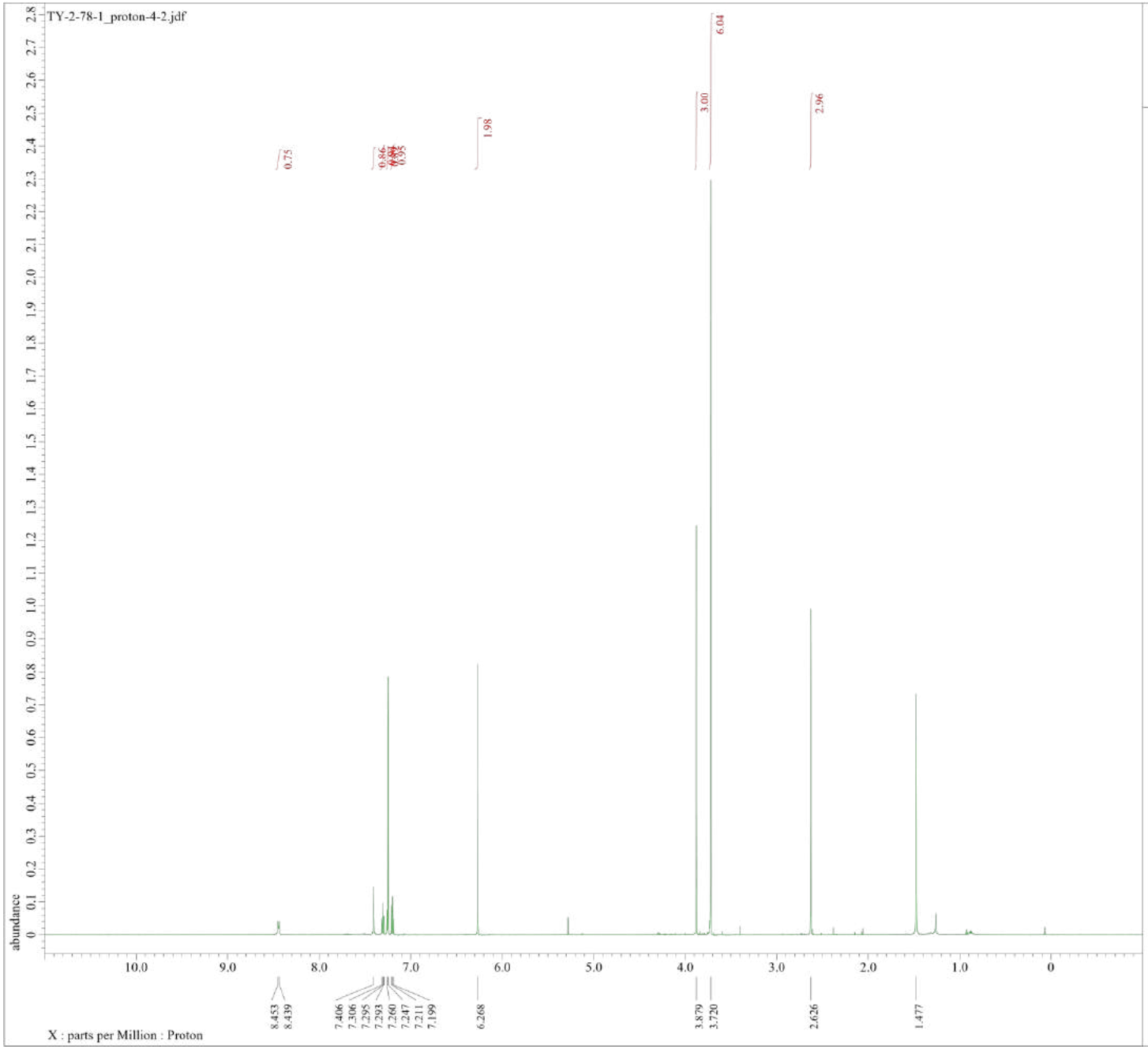
5ja



Filename	= TY-2-130-3_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-130-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-AUG-2021 21:46:
Revision_Time	= 17-AUG-2021 09:00:
Comment	= Bz A2
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 4096
Total_Scans	= 4096
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



5ja



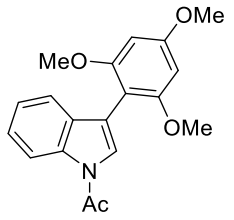
JEOL

```
Filename              = TY-2-78-1_proton-4-2.
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-78-1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 21-SEP-2021 21:40:56
Revision_Time         = 22-SEP-2021 09:12:08

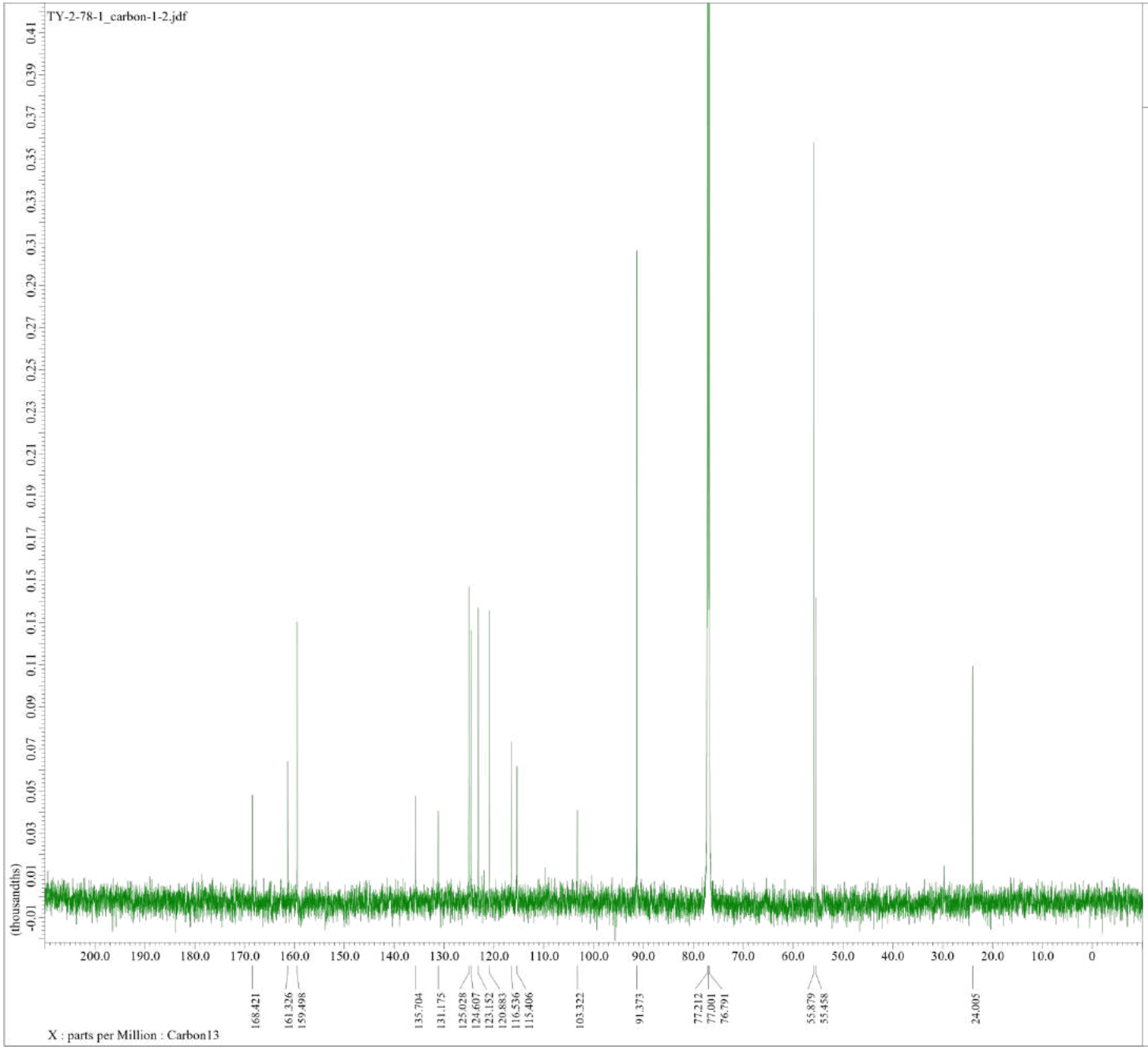
Comment               = Ac triOMe
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

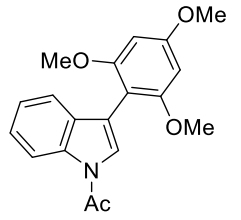
Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 50[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = (0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



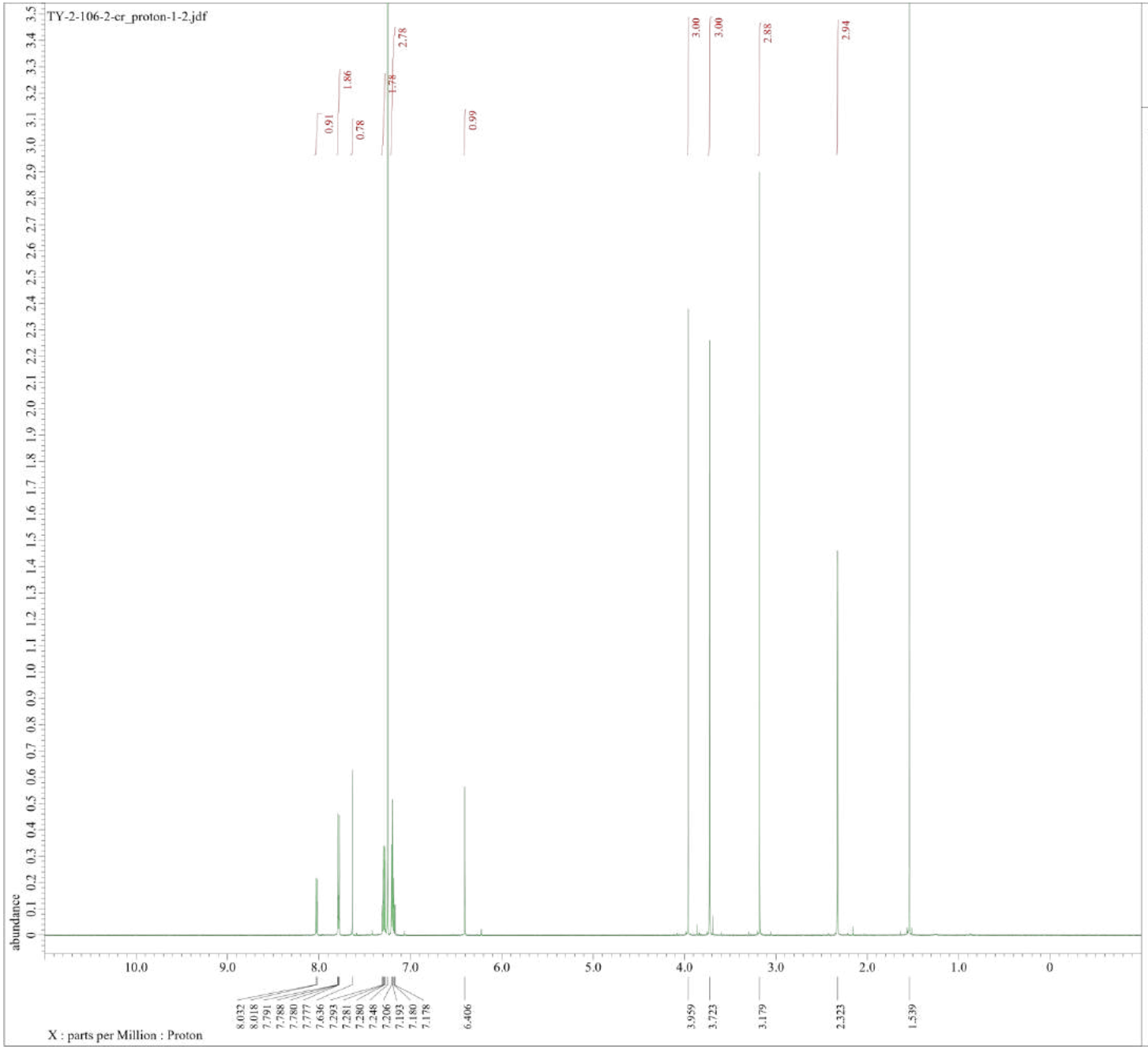
5ka



Filename	= TY-2-78-1_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-78-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-SEP-2021 21:42:
Revision_Time	= 22-SEP-2021 09:08:
Comment	= Ac triOMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8192
Total_Scans	= 8192
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 50[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



5ka



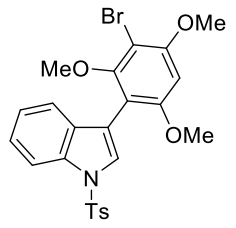
JEOL

```
Filename              = TY-2-106-2-cr_proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-106-2-cr
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  4-AUG-2021 17:42:56
Revision_Time         =  4-AUG-2021 18:06:19

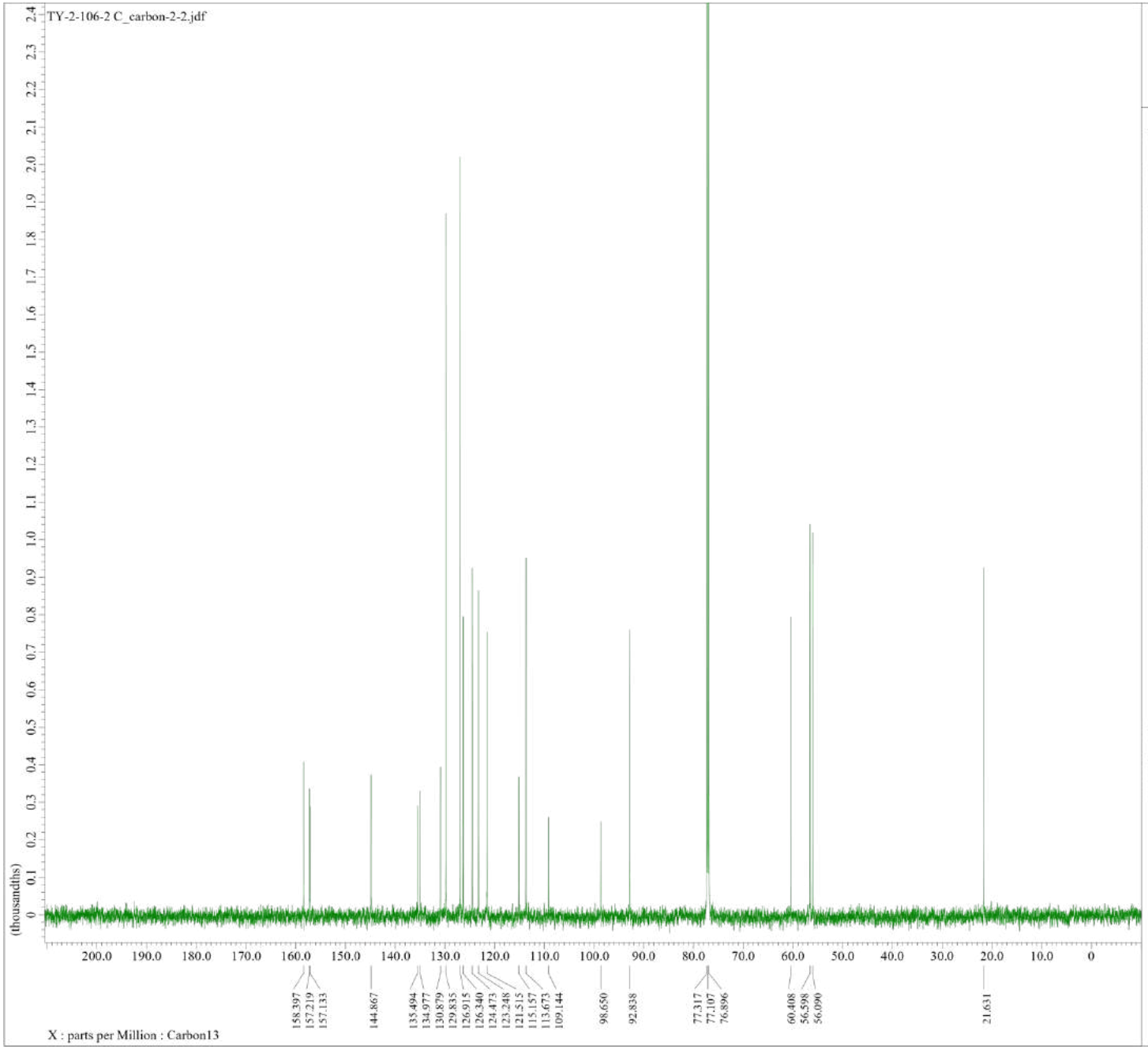
Comment               = Br triOMe AZ
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 66
Temp_Get              = 21.2[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

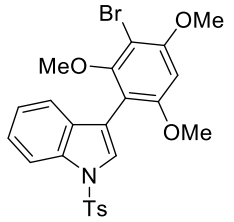


5ab

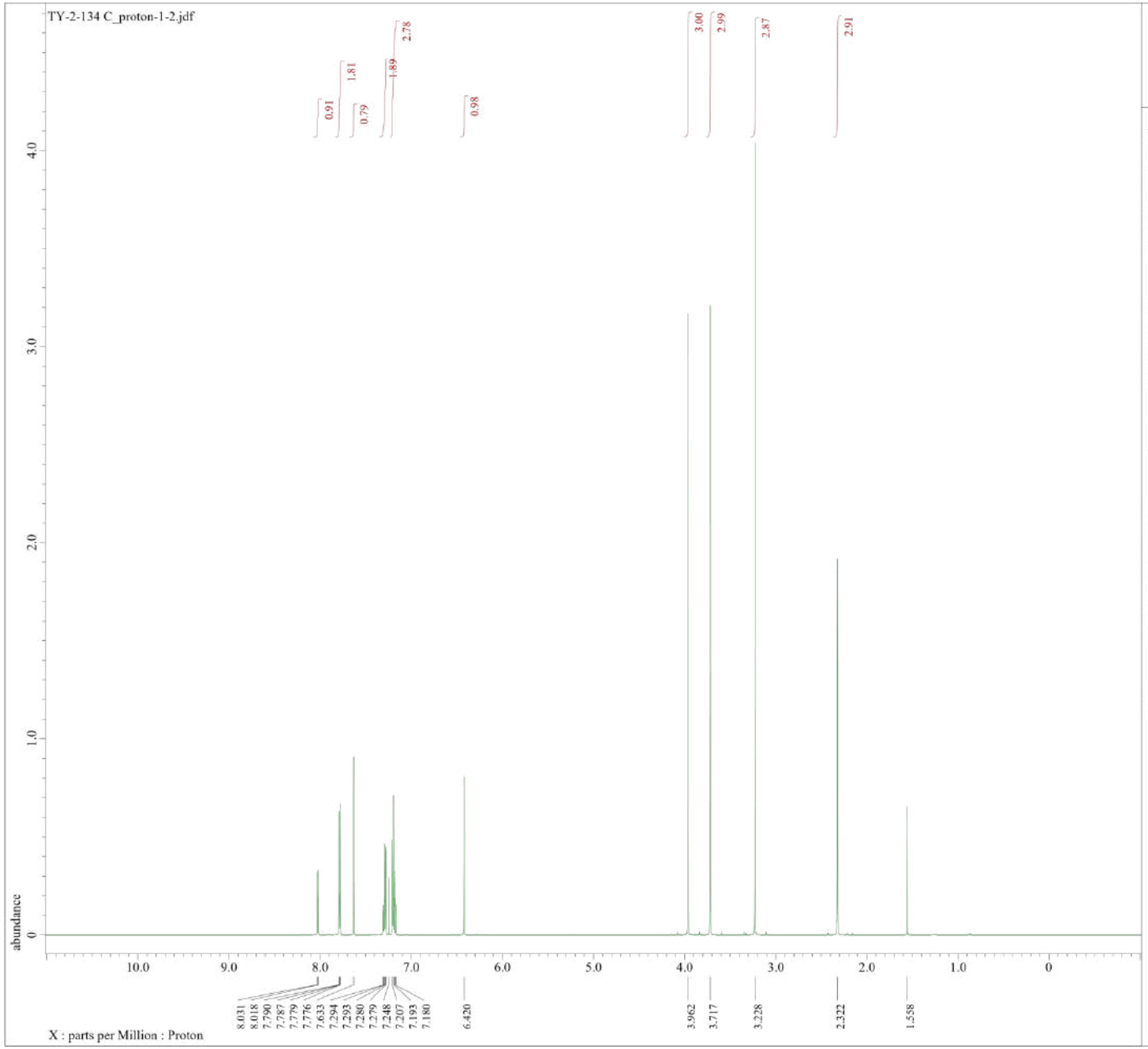


JEOL

Filename	= TY-2-106-2 C_carbo
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-106-2 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-AUG-2021 20:56:
Revision_Time	= 7-AUG-2021 08:41:
Comment	= triOMe Br
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



5ab



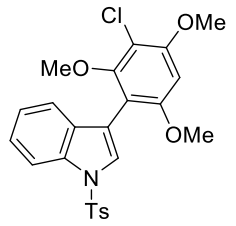
JEOL

```
Filename              = TY-2-134 C_proton-1-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-134 C
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 24-AUG-2021 21:32:01
Revision_Time         = 24-AUG-2021 21:36:05

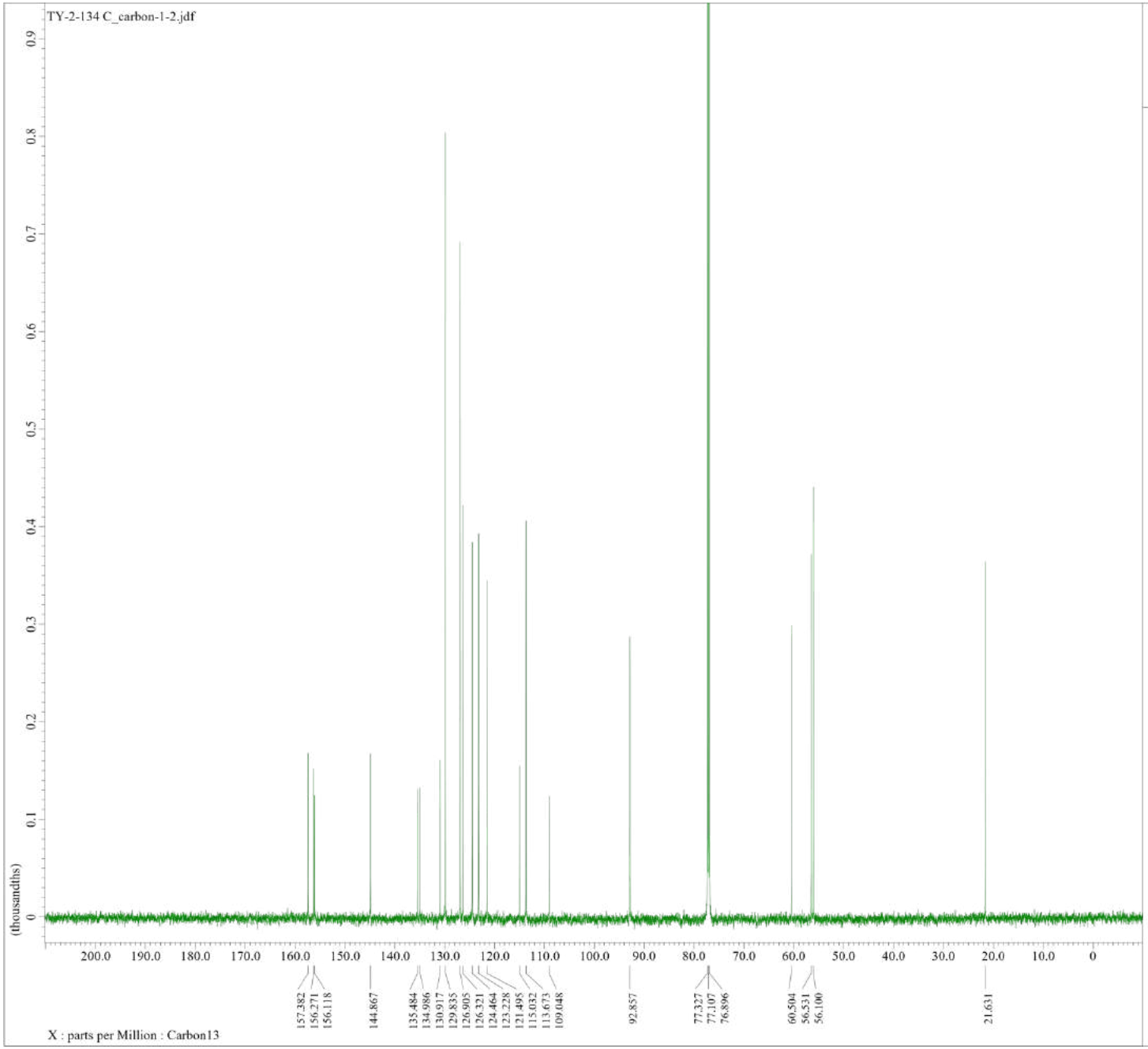
Comment               = triOMe Cl
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 46
Temp_Get              = 20.9[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

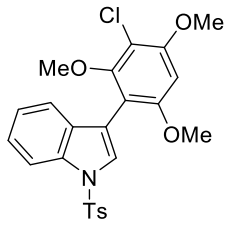


5ac

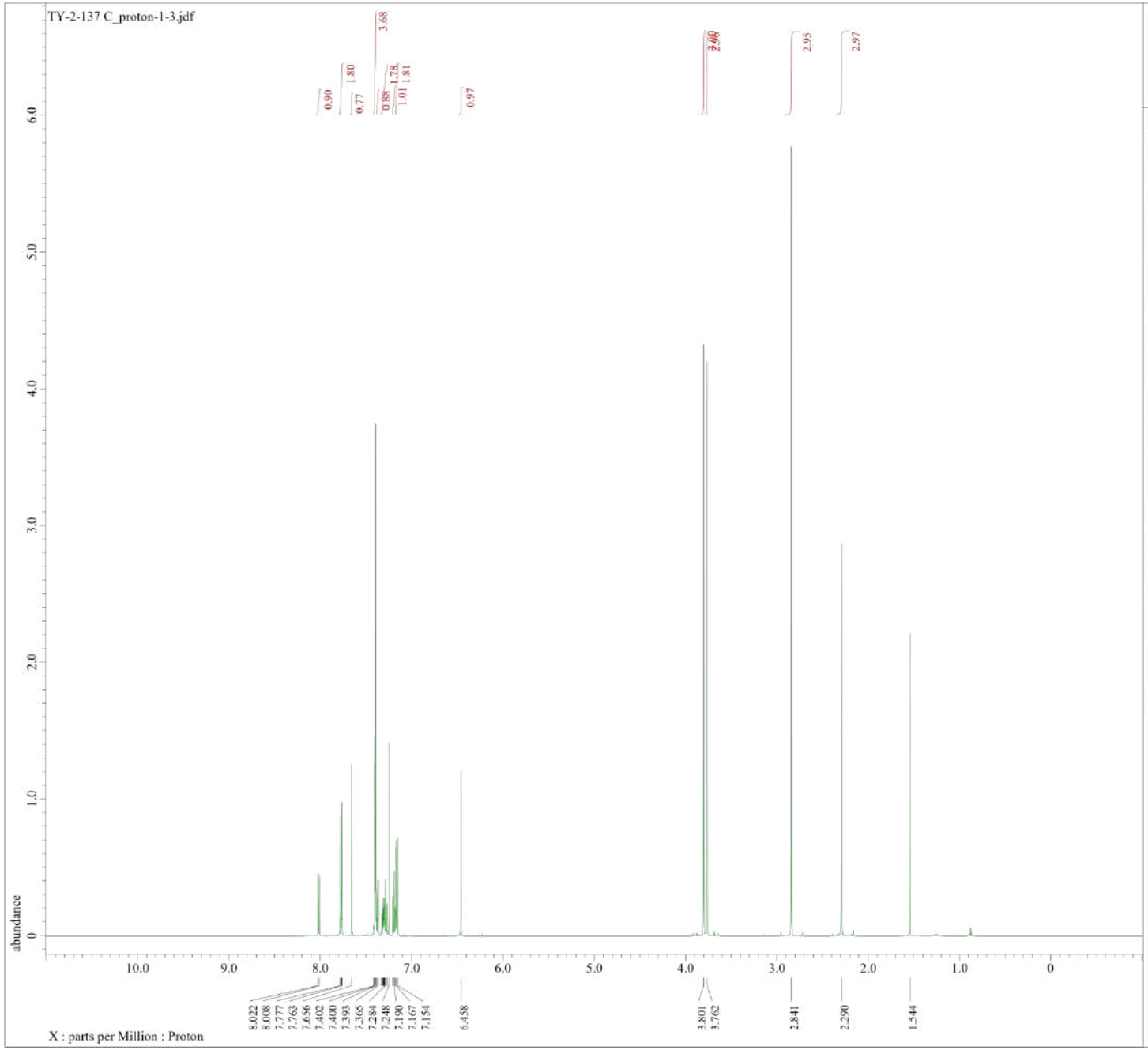


JEOL

Filename	= TY-2-134 C_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-134 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-AUG-2021 22:53:
Revision_Time	= 25-AUG-2021 08:36:
Comment	= triOMe Cl
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 2048
Total_Scans	= 2048
Relaxation_Delay	= 1[s]
Recvr_Gain	= 26
Temp_Get	= 21[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

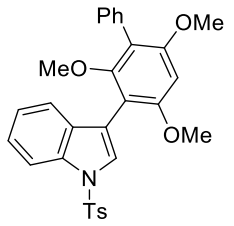


5ac

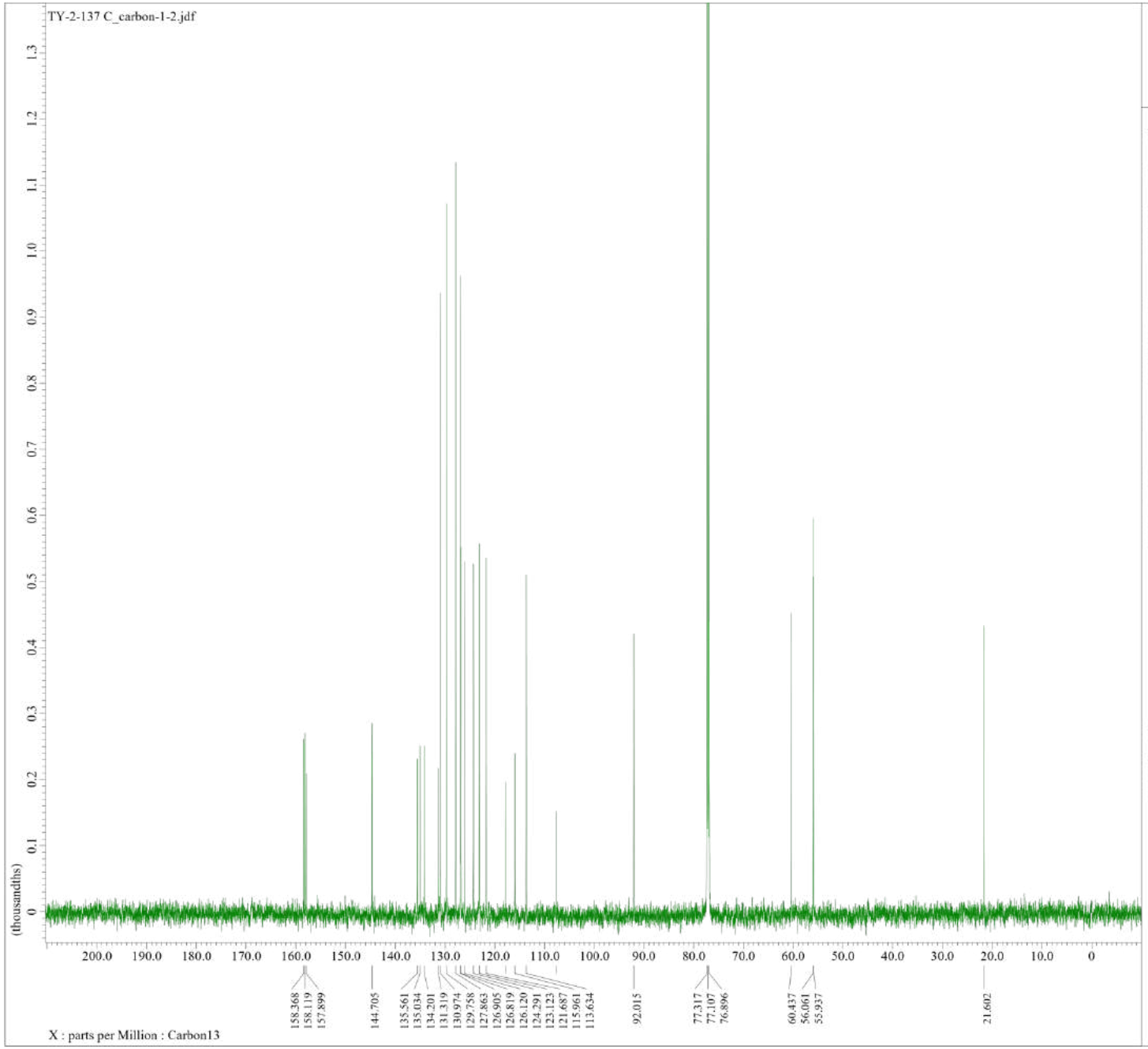


JEOL

Filename	= TY-2-137 C_proton-1-3
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-137 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-AUG-2021 21:27:40
Revision_Time	= 24-AUG-2021 21:33:41
Comment	= triOMe Ph
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

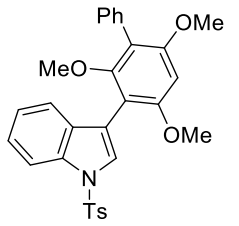


5ad



JEOL

Filename	= TY-2-137 C_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-137 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-AUG-2021 21:38:
Revision_Time	= 25-AUG-2021 08:37:
Comment	= triOMe Ph
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1979
Total_Scans	= 1979
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



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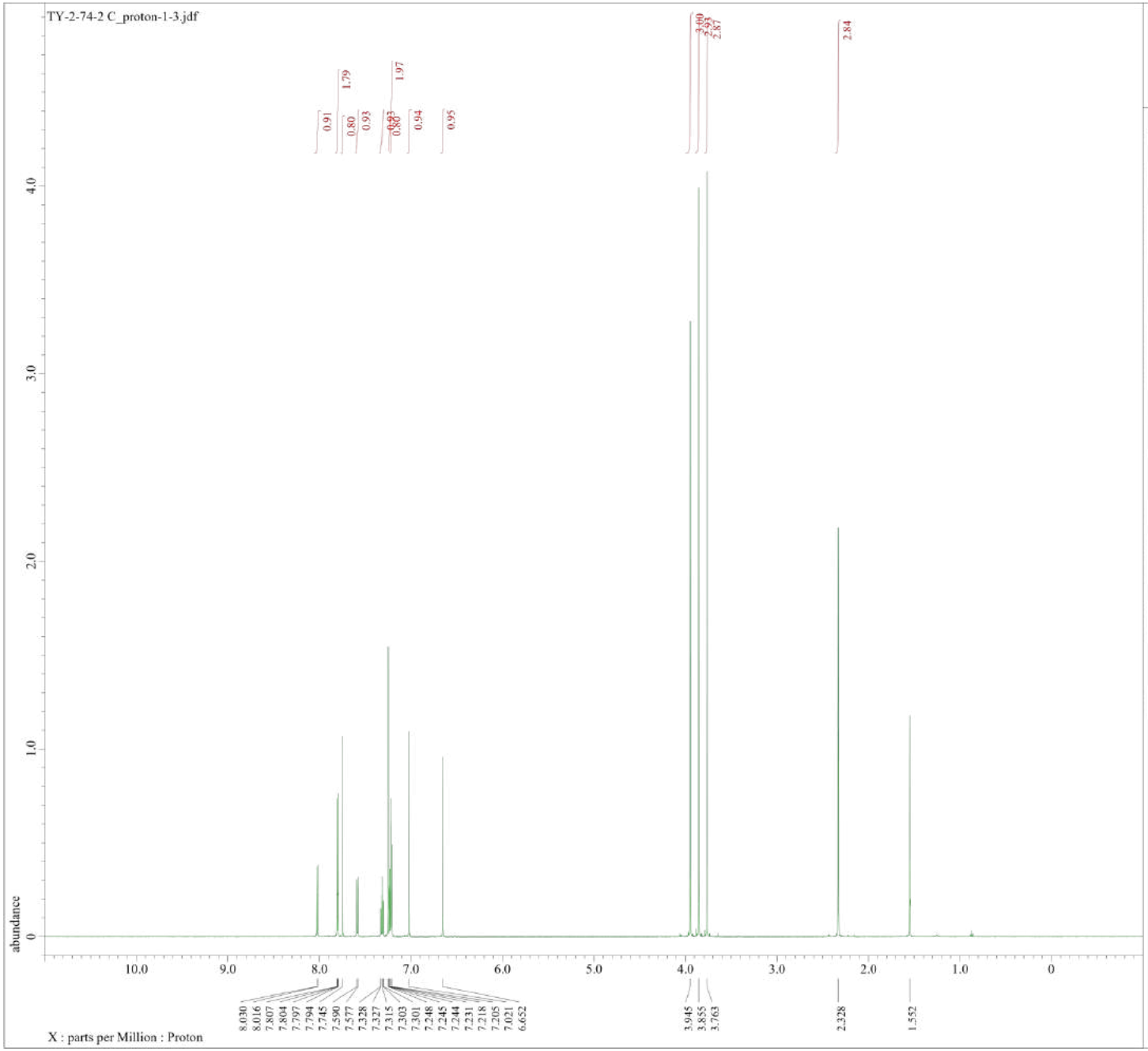
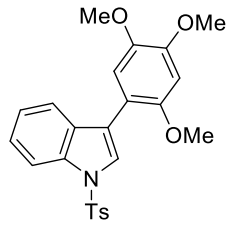



```
Filename              = TY-2-74-2 C_proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-74-2 C
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  6-AUG-2021 20:46:16
Revision_Time         =  6-AUG-2021 20:57:16

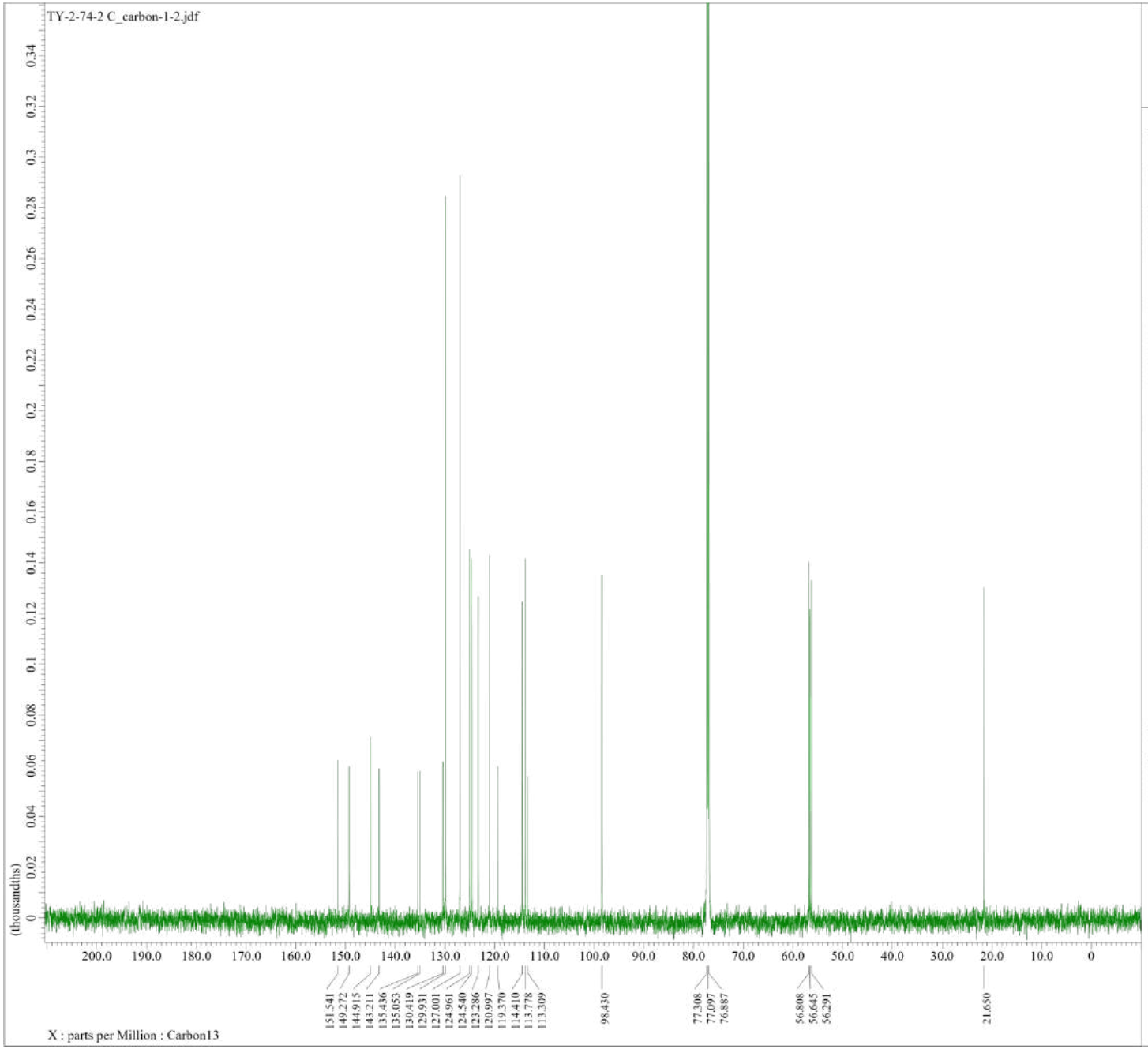
Comment               = 1,2,4-triOMe
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 21[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```

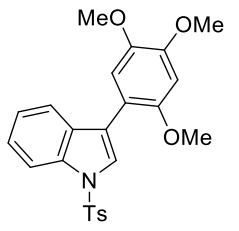



5ae

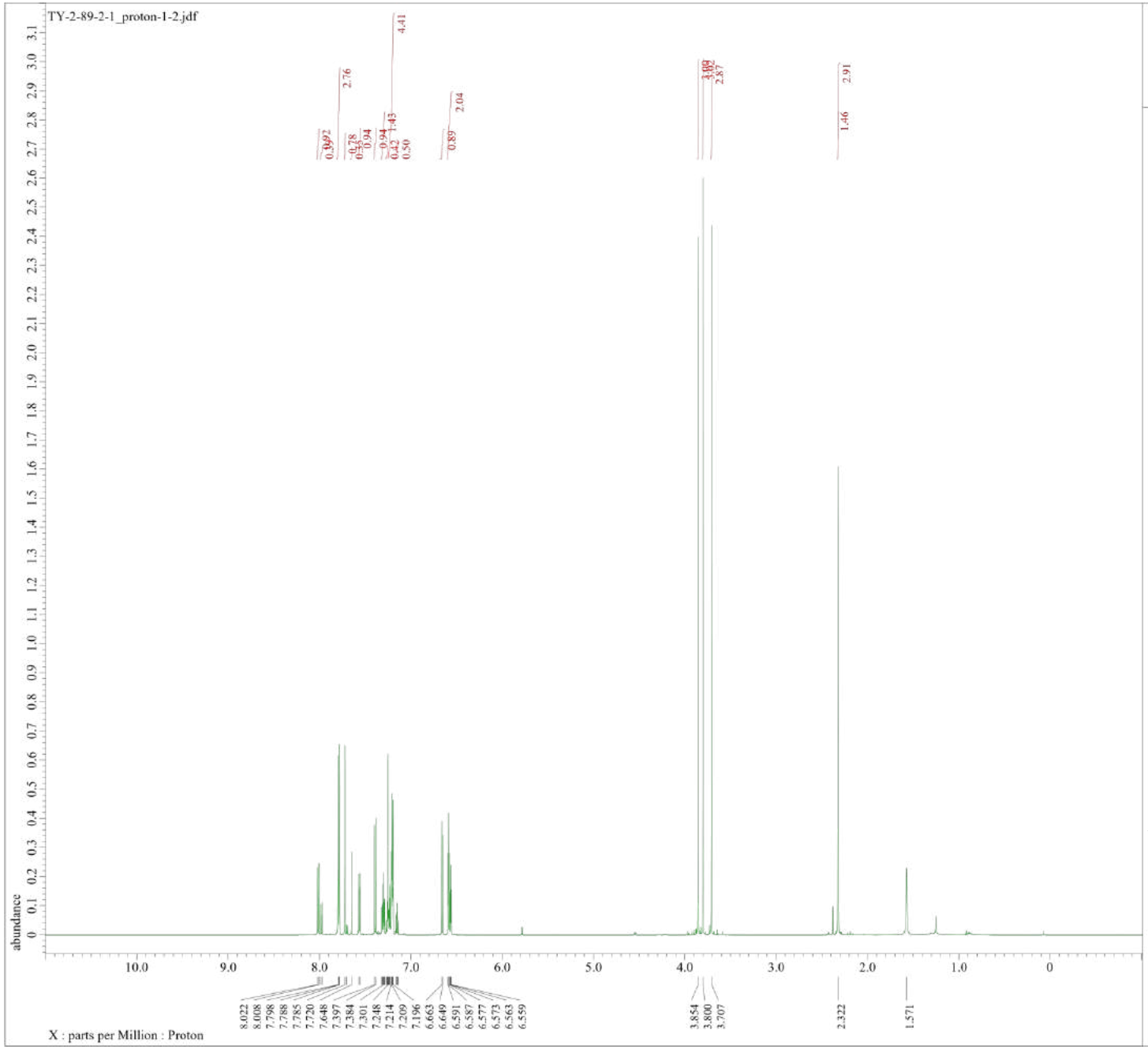


JEOL

Filename	= TY-2-74-2 C_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-74-2 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-AUG-2021 21:36:
Revision_Time	= 7-AUG-2021 08:44:
Comment	= 1,2,4-triOMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 4096
Total_Scans	= 4096
Relaxation_Delay	= 1[s]
Recvr_Gain	= 26
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

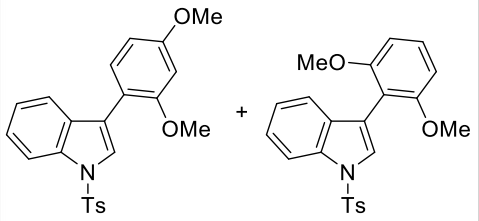


5ae



JEOL

Filename	= TY-2-89-2-1_proton-1-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-89-2-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-AUG-2021 20:11:21
Revision_Time	= 2-AUG-2021 20:38:29
Comment	= 1,3-diOMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 46
Temp_Get	= 21.1[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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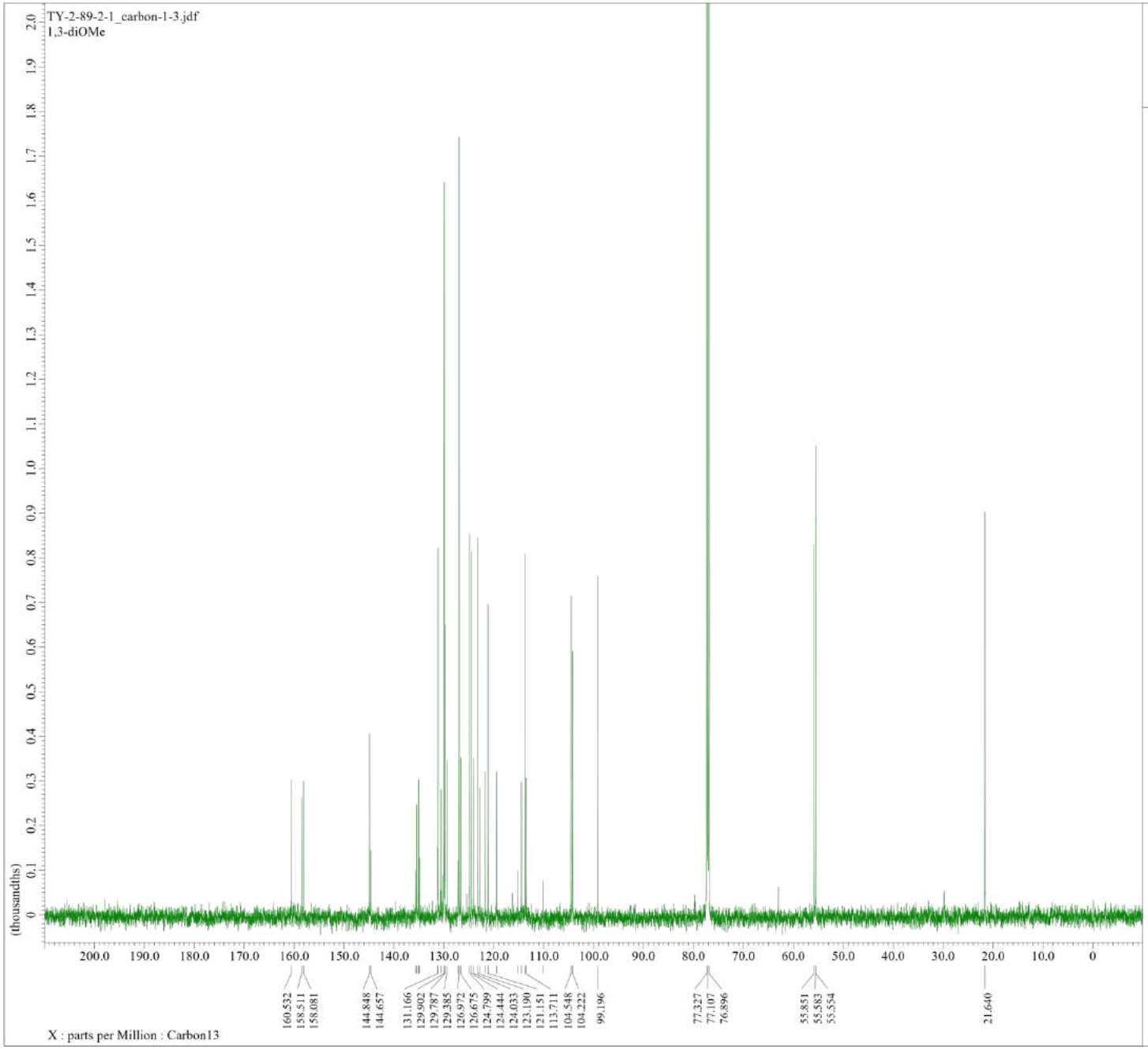
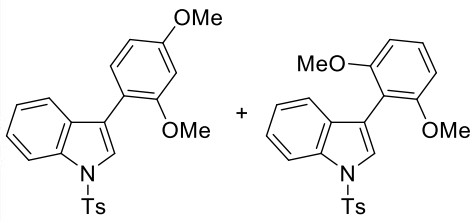


JEOL

Filename	= TY-2-89-2-1_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-89-2-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-AUG-2021 20:49:
Revision_Time	= 8-OCT-2021 19:11:
Comment	= 1,3-diOMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1199
Total_Scans	= 1199
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21.2[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



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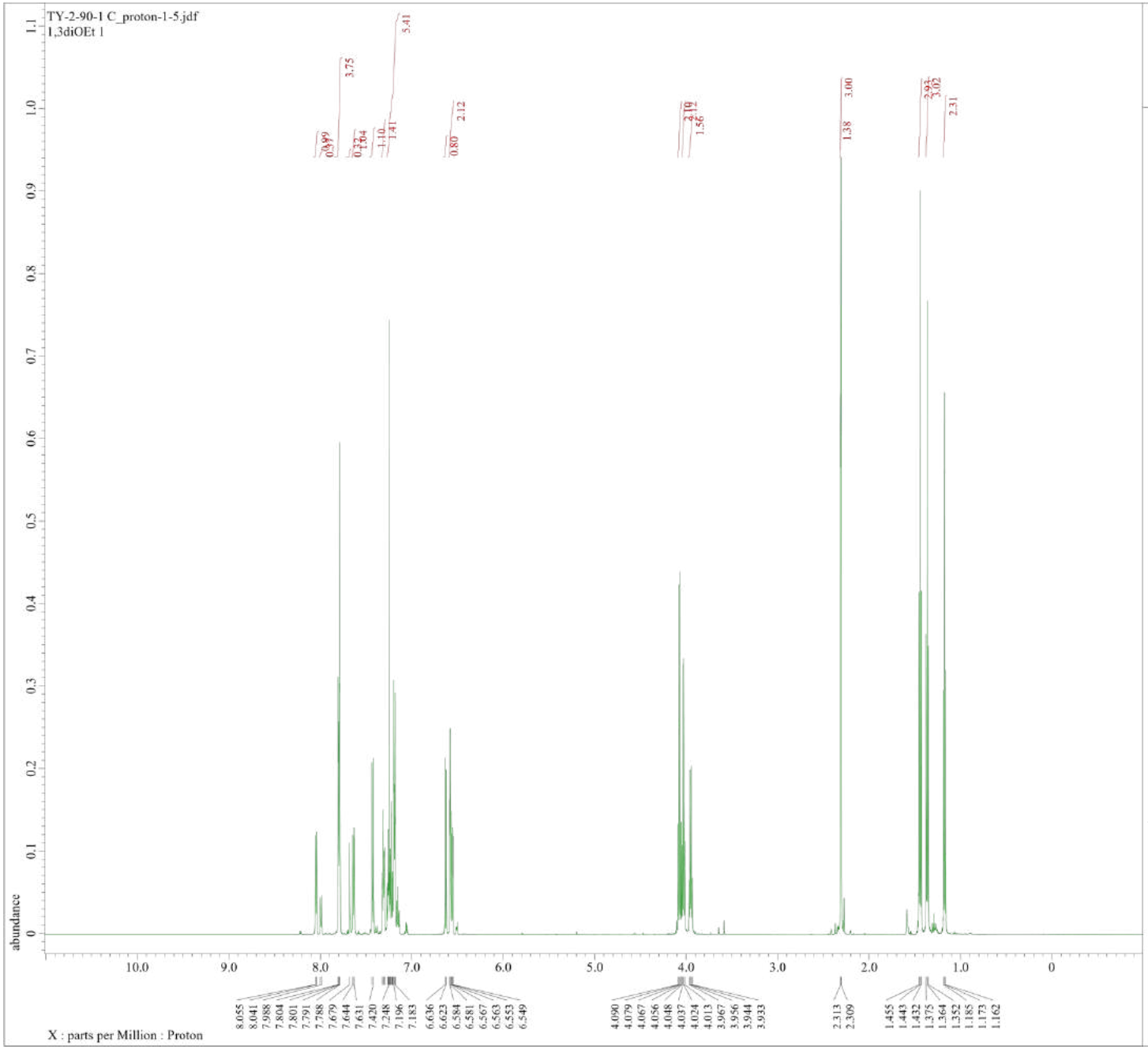


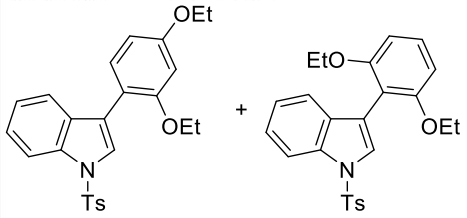
JEOL

```
Filename              = TY-2-90-1 C_proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-90-1 C
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 21-JUL-2021 21:26:10
Revision_Time         = 11-OCT-2021 15:20:18

Comment               = 1,3diOEt 1
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 36
Temp_Get              = 20.8[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



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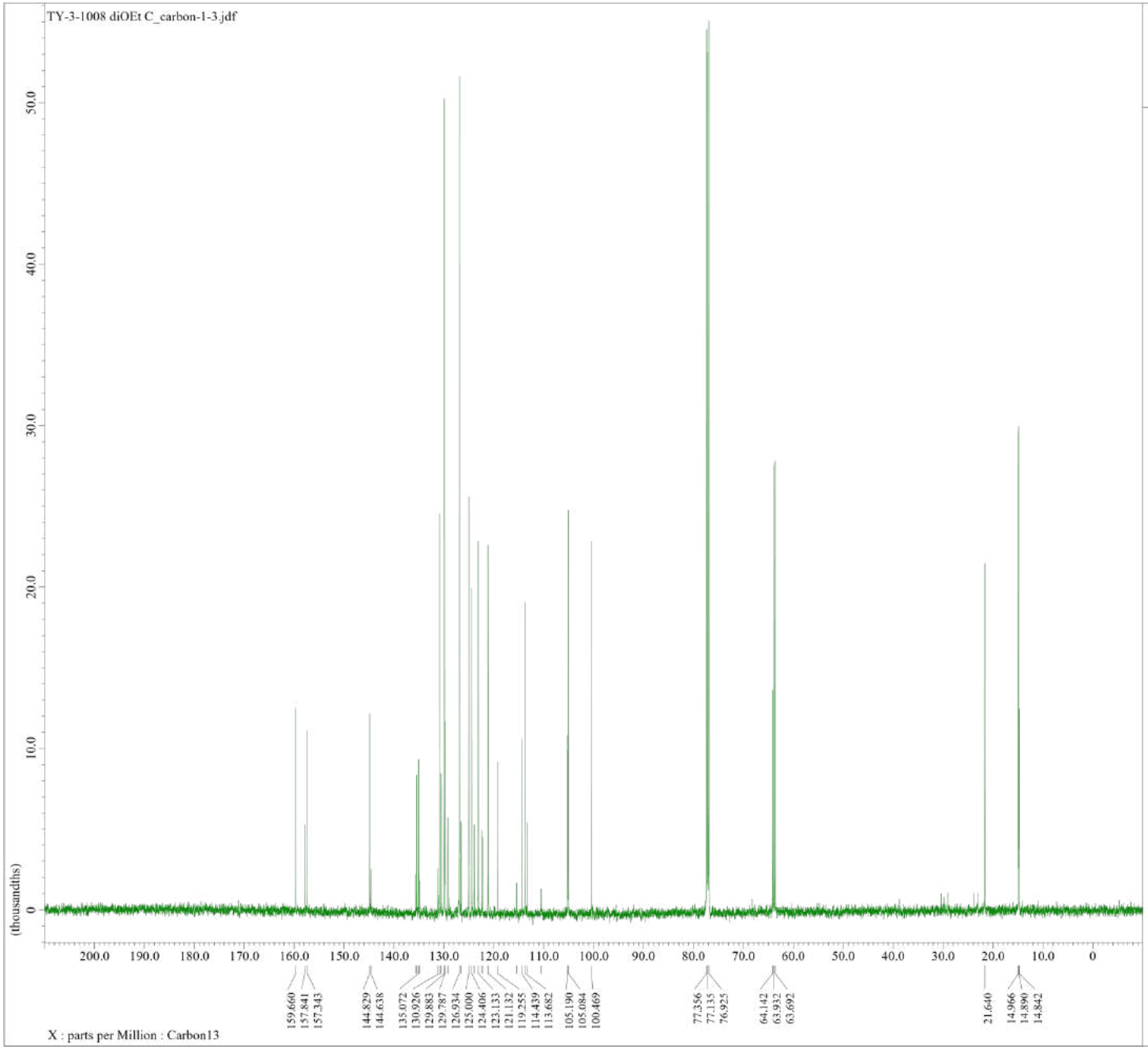
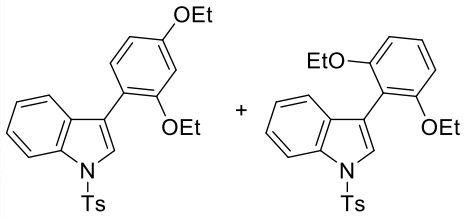


JEOL

Filename	= TY-3-1008 diOEt C_
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-3-1008 diOEt C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-OCT-2021 02:52:
Revision_Time	= 9-OCT-2021 03:03:
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15[us]
Clipped	= FALSE
Scans	= 130
Total_Scans	= 130
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[dC]
X_90_Width	= 9.6[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 3.2[us]
Irr_Atn_Dec	= 26.254[dB]
Irr_Atn_Dec_Calc	= 26.254[dB]
Irr_Atn_Dec_Default_Calc	= 26.254[dB]
Irr_Atn_Noe	= 26.254[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



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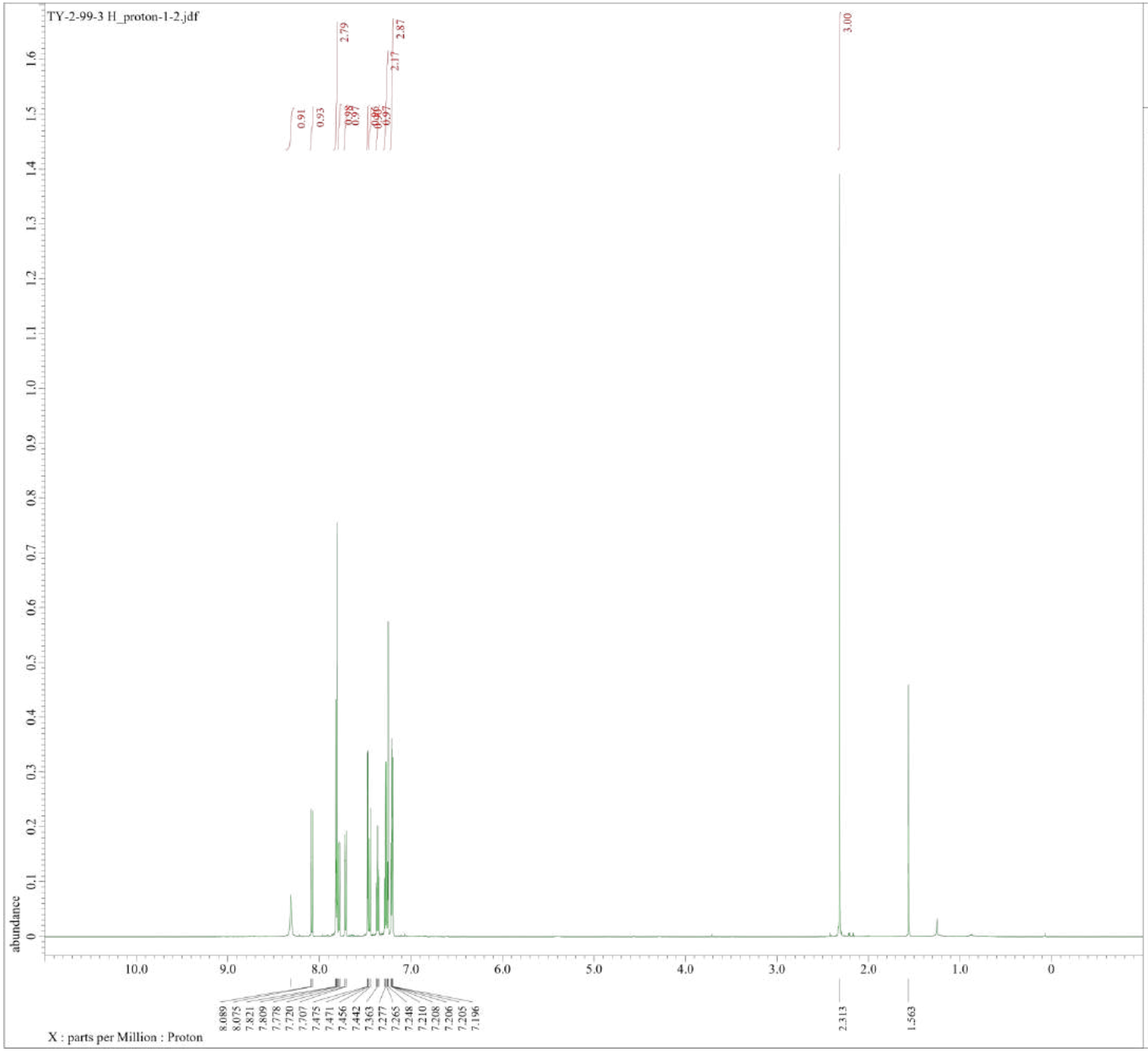


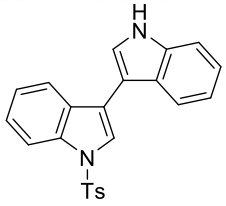
JEOL

```
Filename              = TY-2-99-3 H_proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-99-3 H
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 19-AUG-2021 18:42:50
Revision_Time         = 19-AUG-2021 18:54:02

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

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 46
Temp_Get              = 21[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



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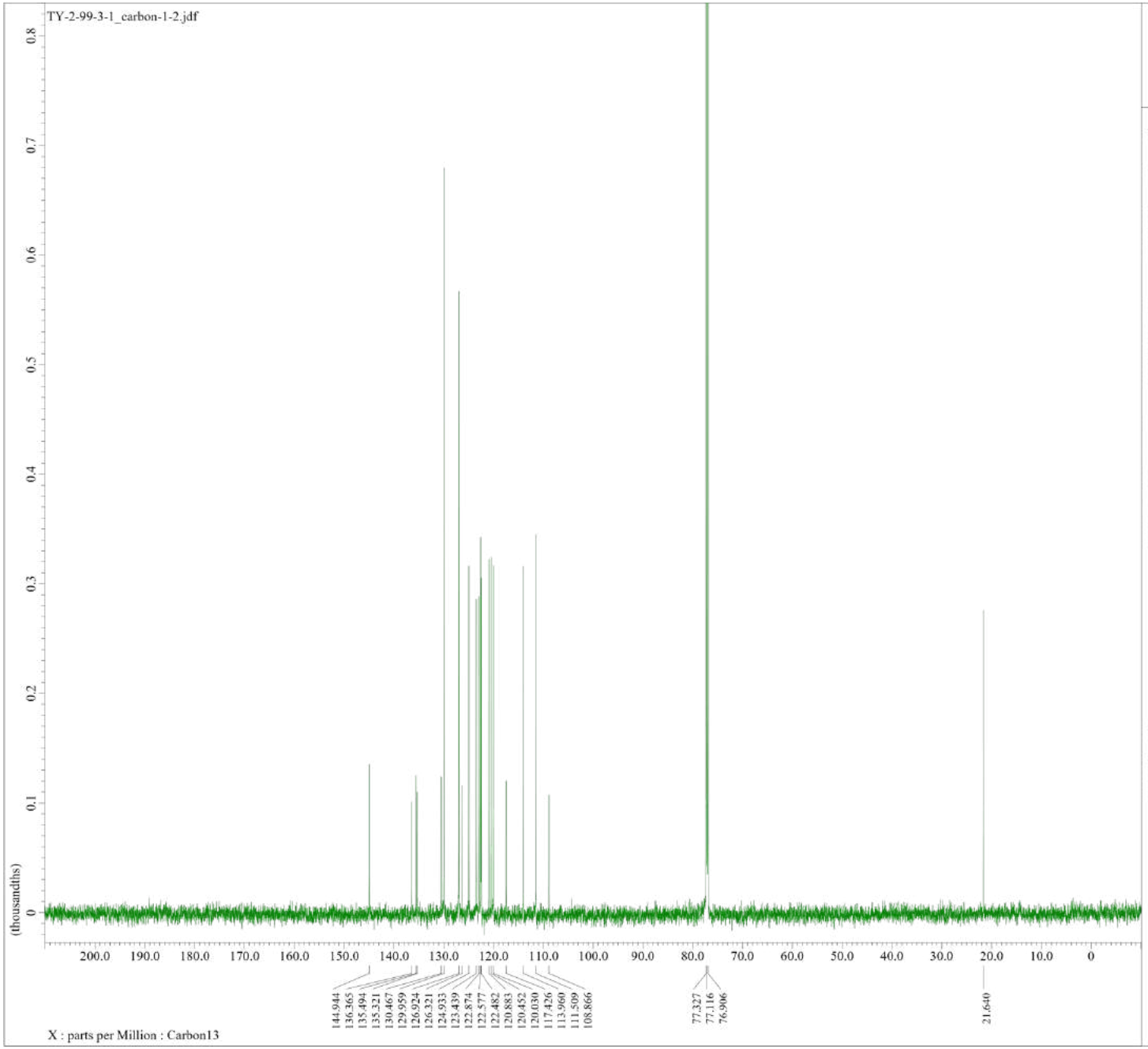
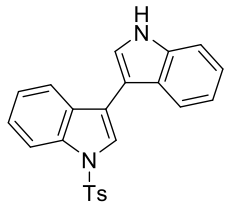
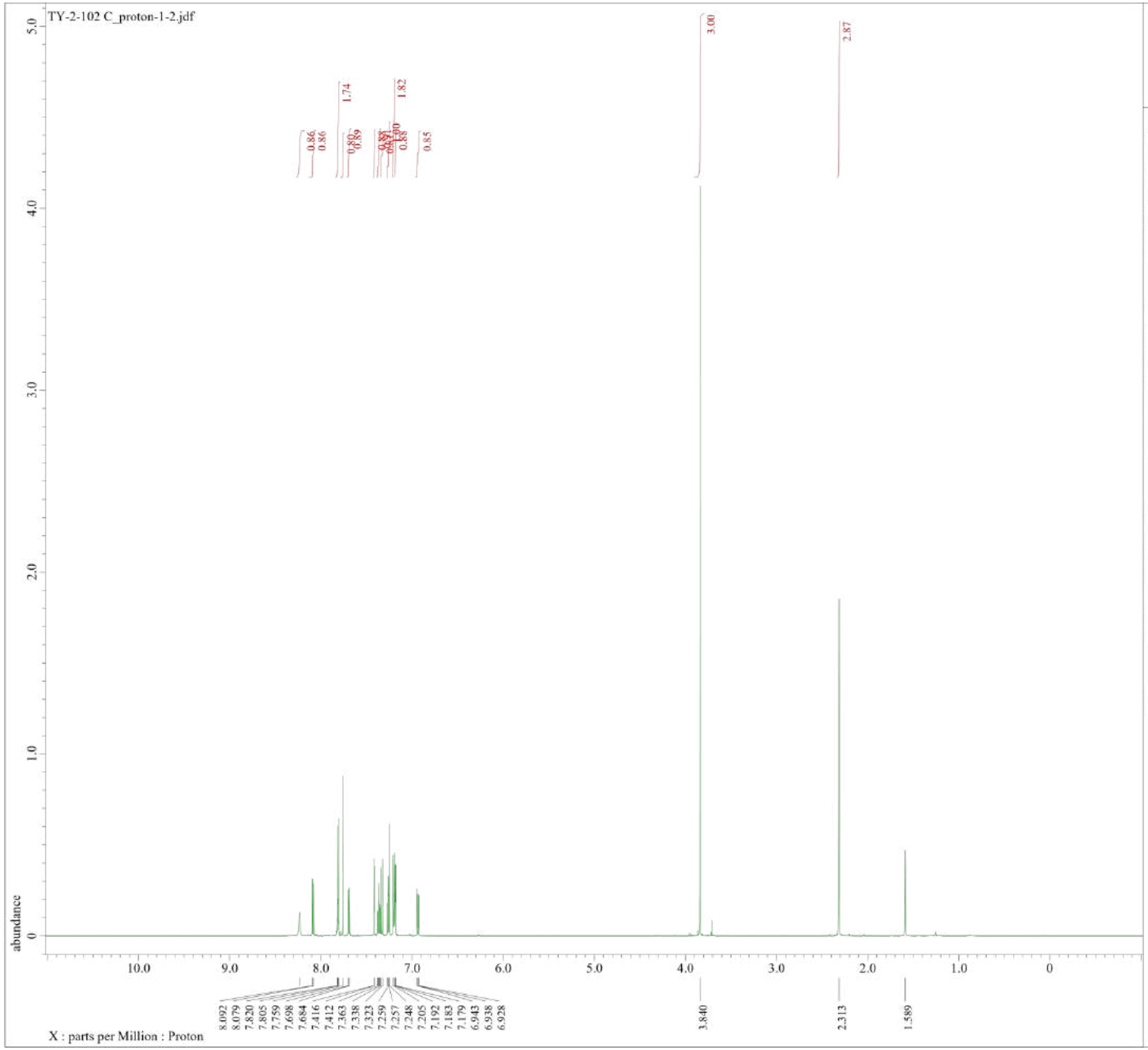


JEOL

Filename	= TY-2-99-3-1_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-99-3-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-AUG-2021 22:14:
Revision_Time	= 19-AUG-2021 19:09:
Comment	= indole AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 26
Temp_Get	= 21.2[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



5ah

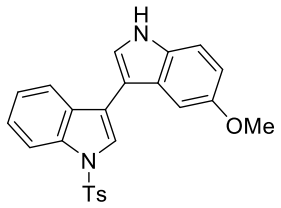



```
Filename              = TY-2-102 C_proton-1-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-102 C
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 21-JUL-2021 21:35:28
Revision_Time         = 17-AUG-2021 14:10:40

Comment               = 5-OMeIN AZ
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 46
Temp_Get              = 20.9[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



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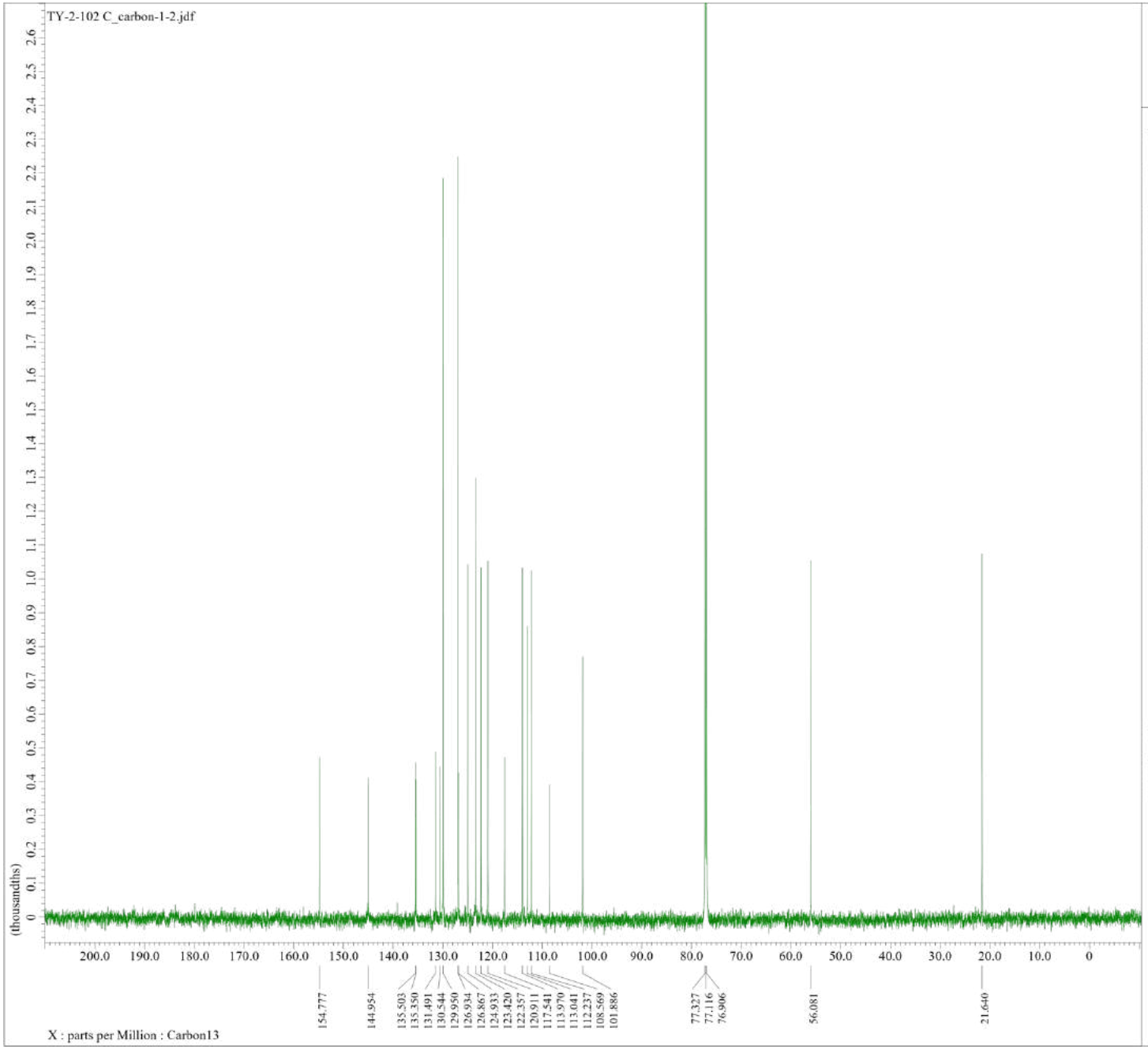
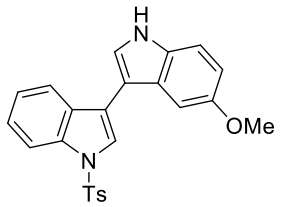
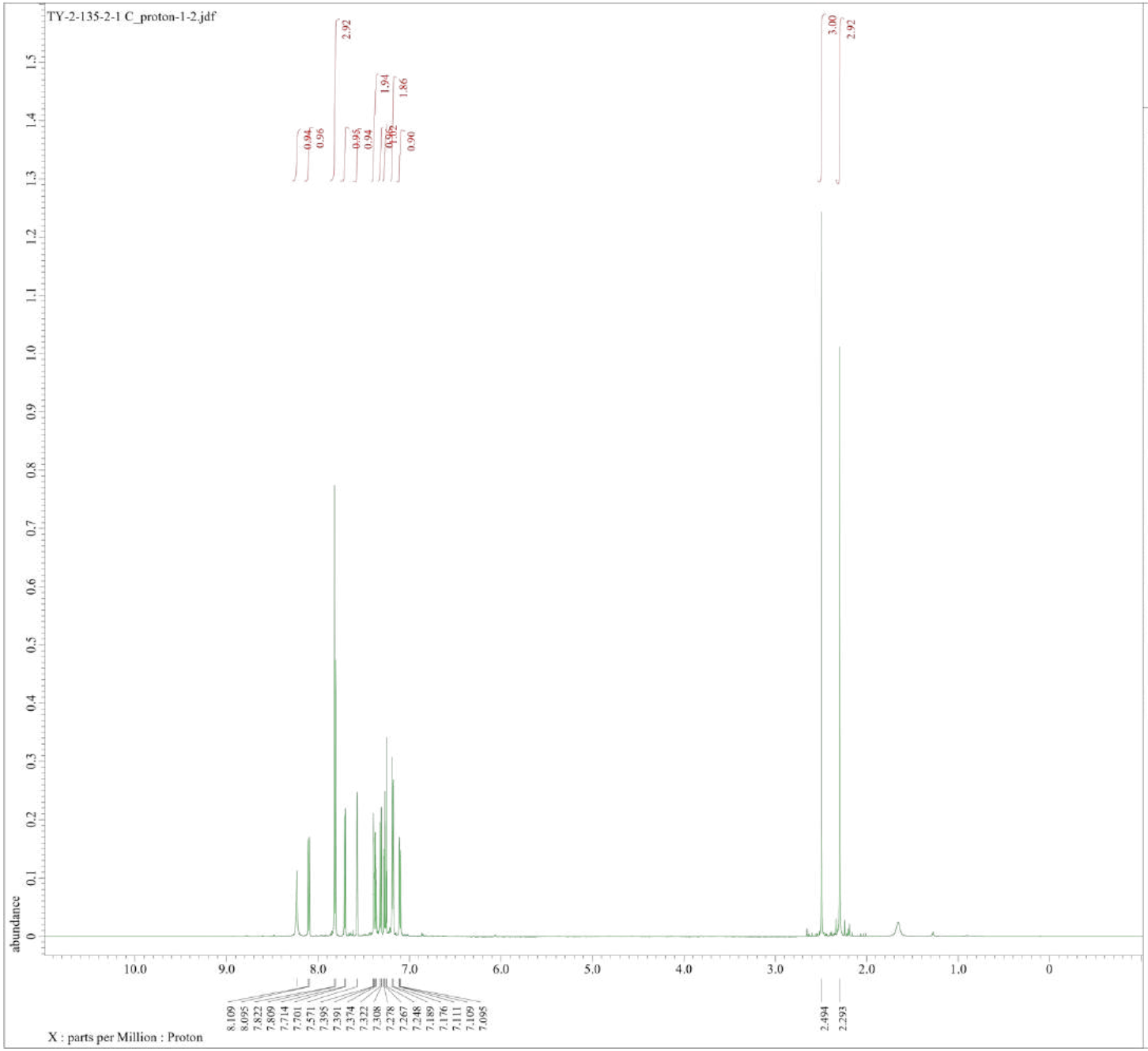


JEOL

Filename	= TY-2-102 C_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-102 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-JUL-2021 23:01:
Revision_Time	= 17-AUG-2021 14:08:
Comment	= 5-OMeIN AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



5ai



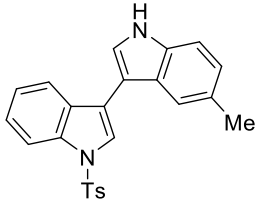
JEOL

```
Filename              = TY-2-135-2-1 C_proton
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-135-2-1 C
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 17-AUG-2021 21:17:26
Revision_Time         = 17-AUG-2021 21:28:52

Comment               = 5-Me indole AZ
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 36
Temp_Get              = 21[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



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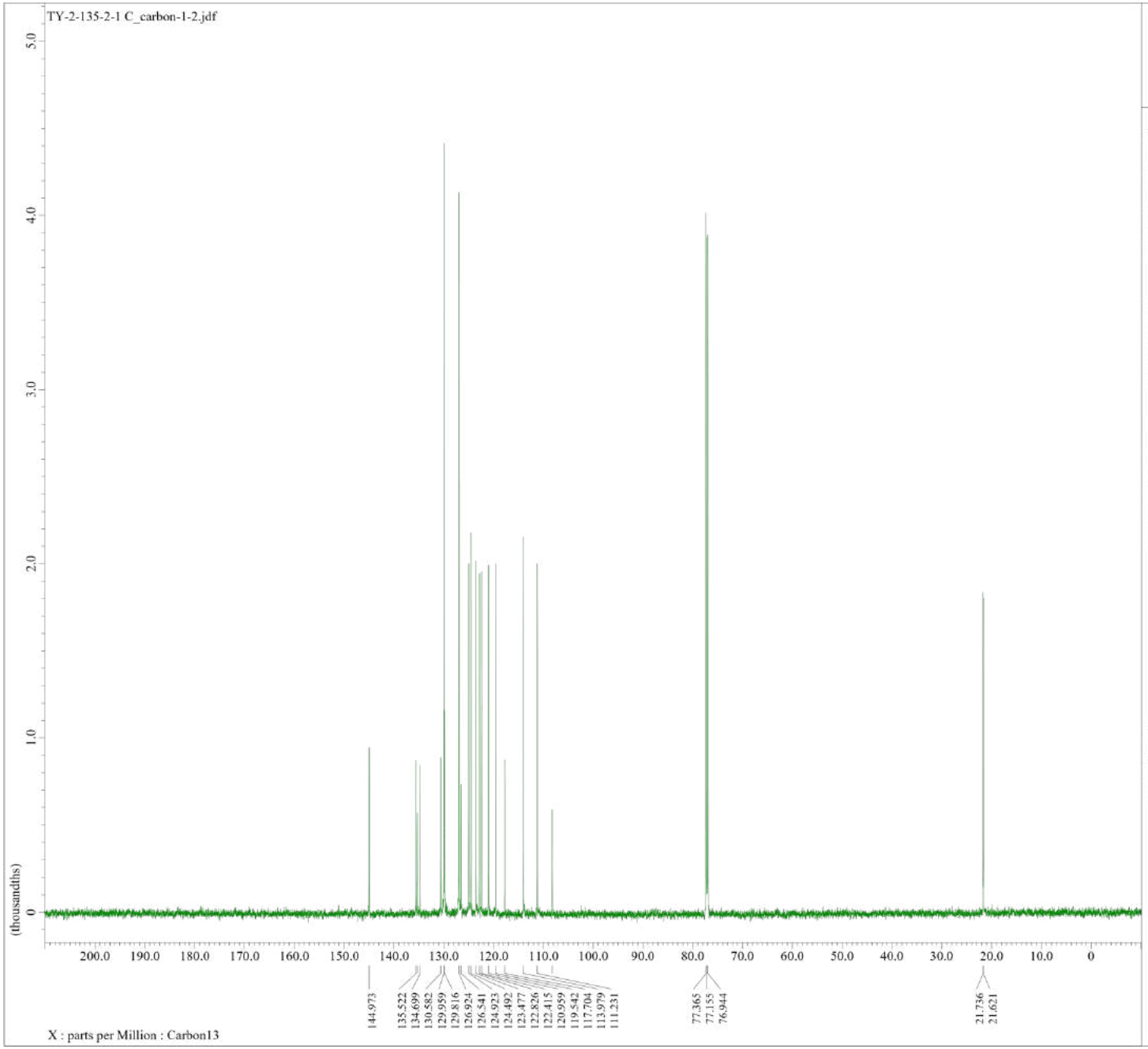
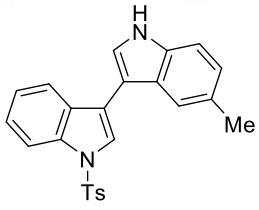


JEOL

Filename	= TY-2-135-2-1 C_car
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-135-2-1 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-AUG-2021 21:37:
Revision_Time	= 20-AUG-2021 21:39:
Comment	= Bs AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 926
Total_Scans	= 926
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



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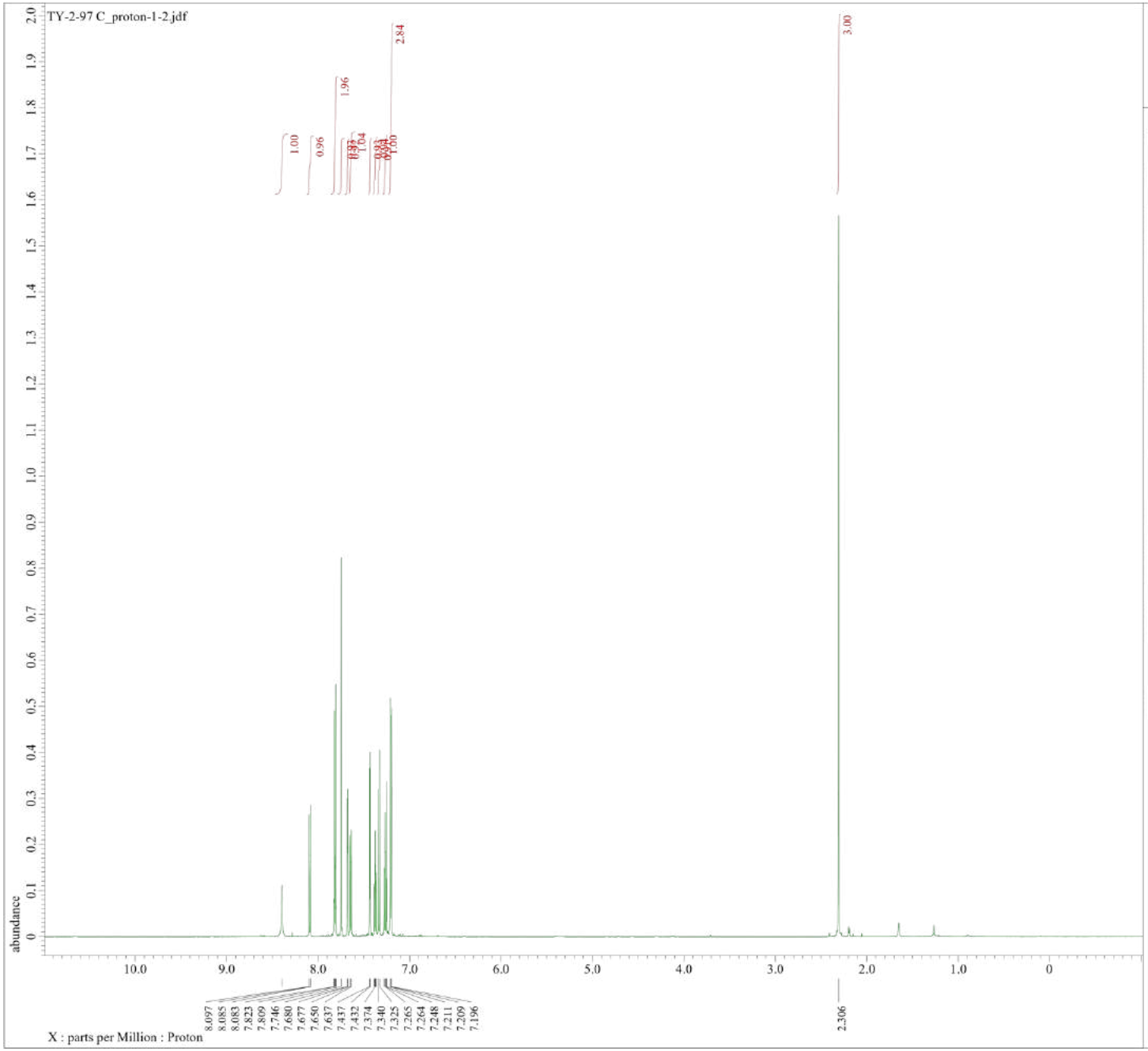
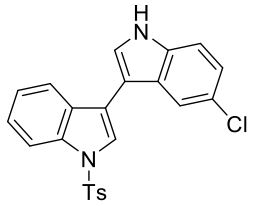



```
Filename              = TY-2-97 C_proton-1-2.
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-97 C
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 21-JUL-2021 21:21:14
Revision_Time         = 17-AUG-2021 14:05:40

Comment               = 5-ClIN
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 36
Temp_Get              = 20.8[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



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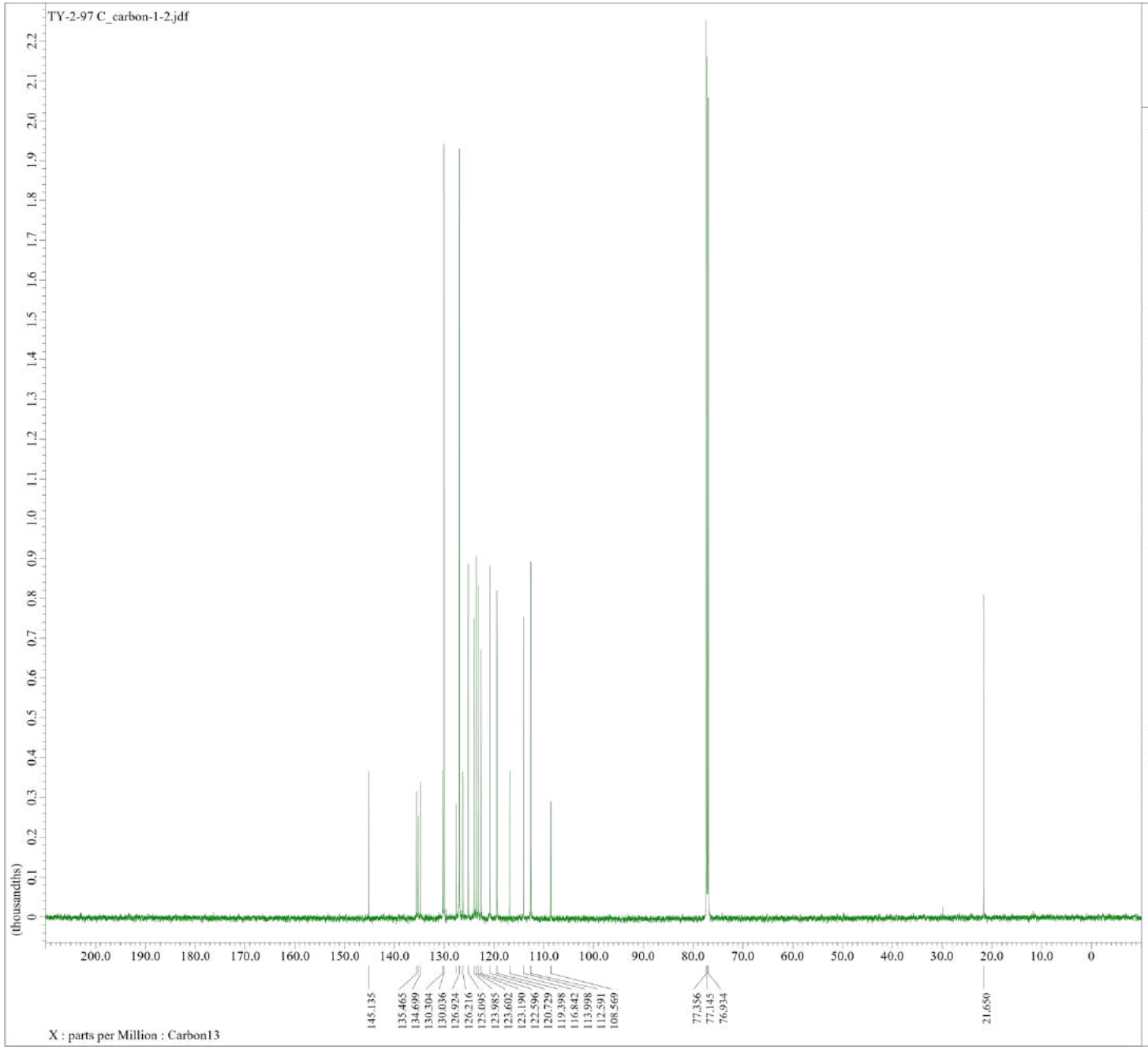
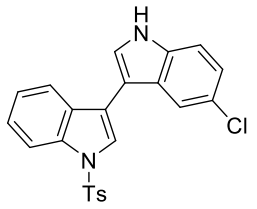


JEOL

Filename	= TY-2-97 C_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-97 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-JUL-2021 22:10:
Revision_Time	= 17-AUG-2021 14:03:
Comment	= 5-ClIN AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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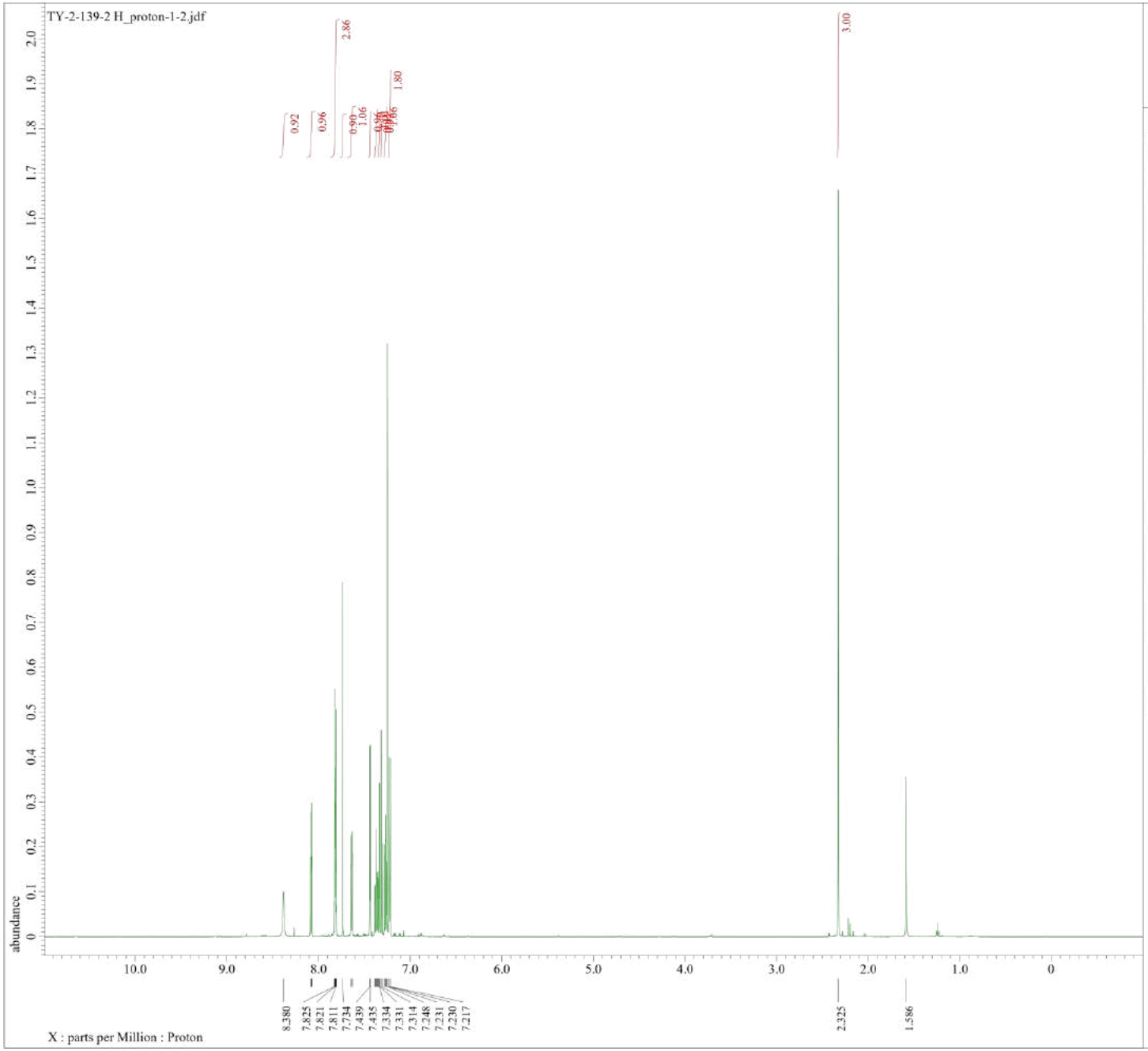
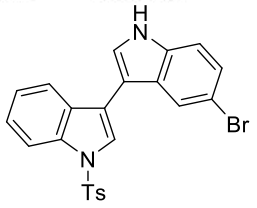


JEOL

Filename	= TY-2-139-2 H_proton-1
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-139-2 H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-AUG-2021 18:54:20
Revision_Time	= 23-AUG-2021 19:35:03
Comment	= 5-Br IN AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 46
Temp_Get	= 20.8[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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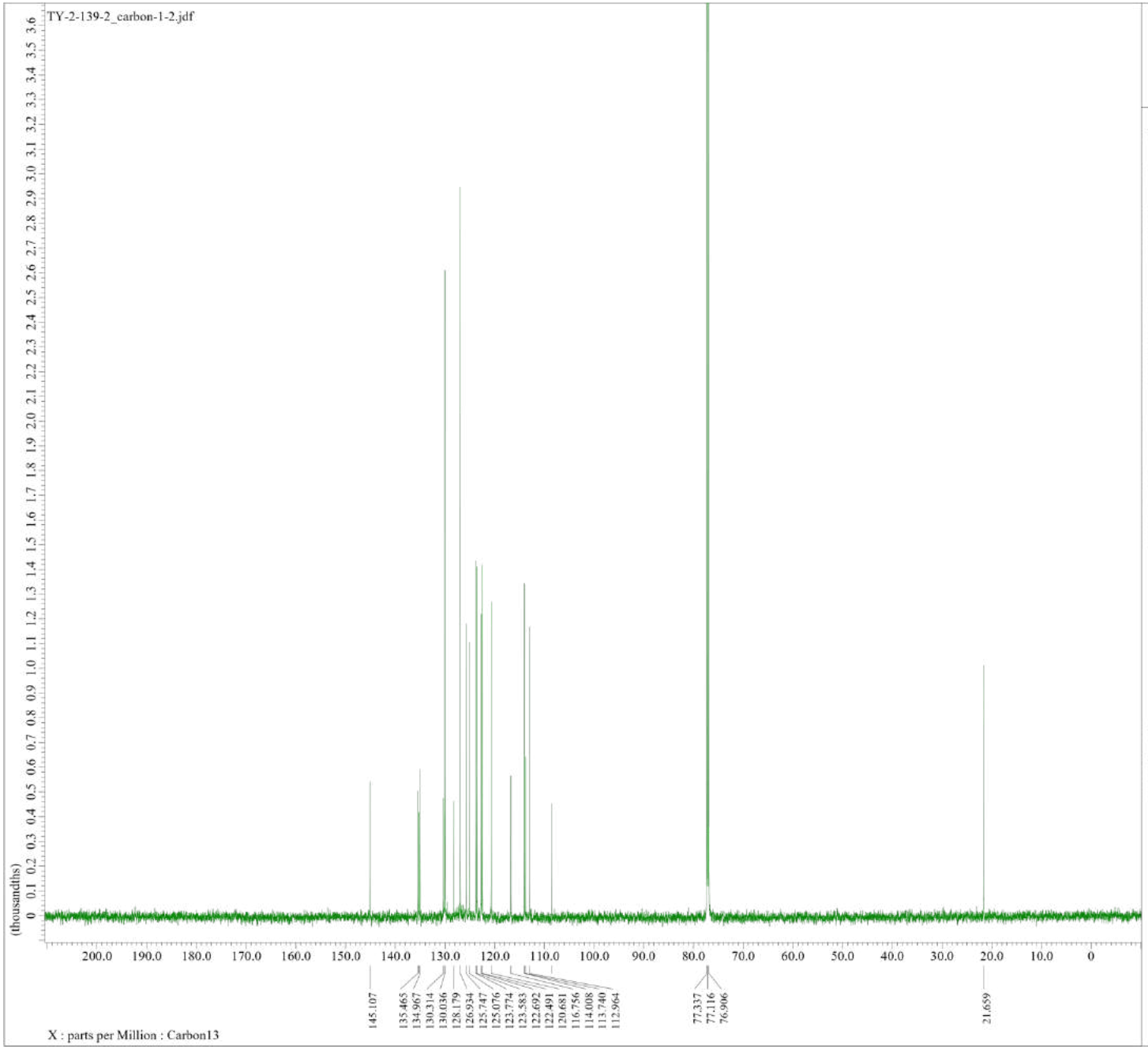
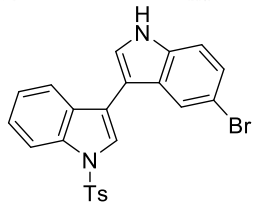
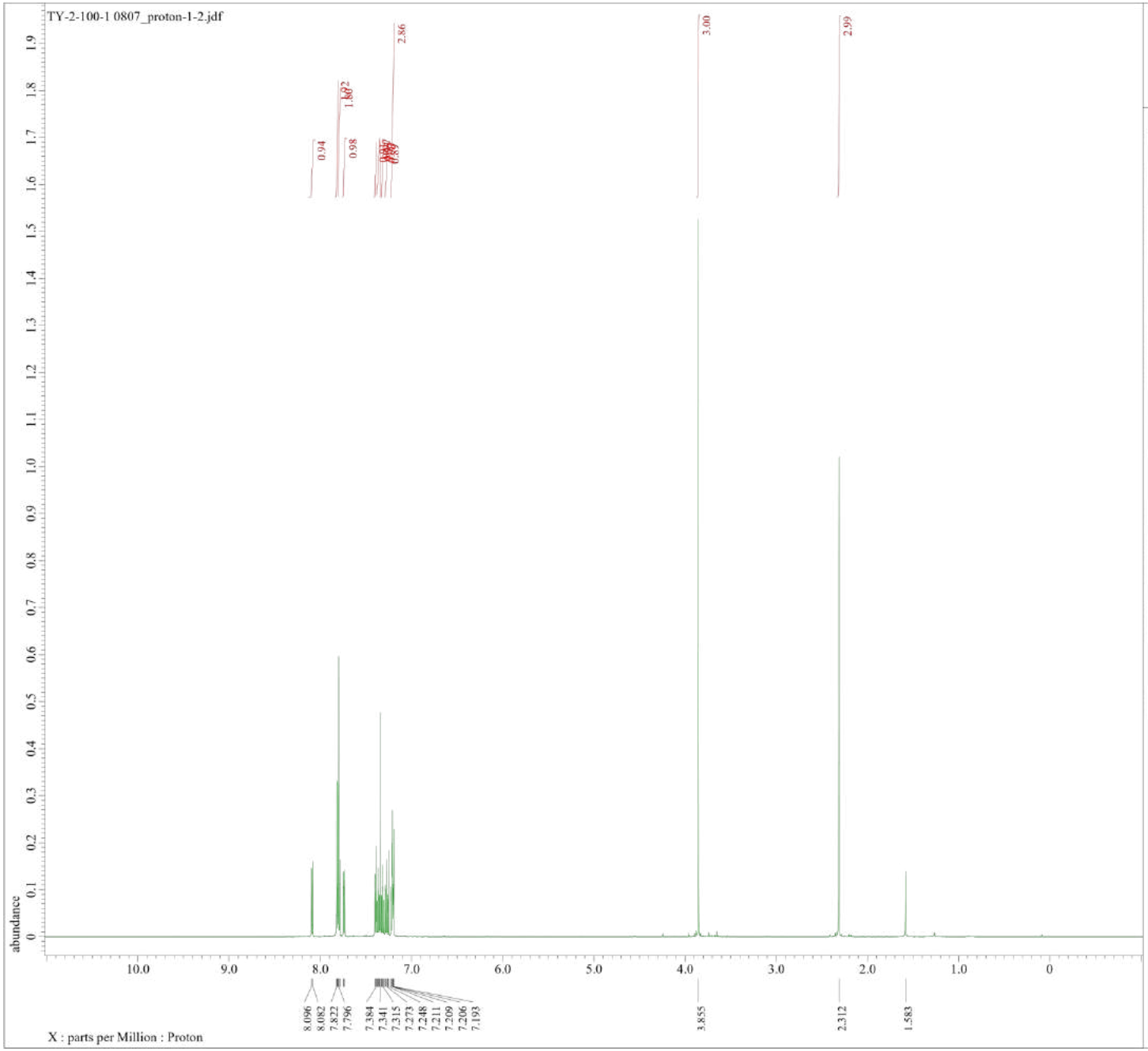


JEOL

Filename	= TY-2-139-2_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-139-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-AUG-2021 22:42:
Revision_Time	= 21-AUG-2021 10:15:
Comment	= 5-Br IN AZ
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

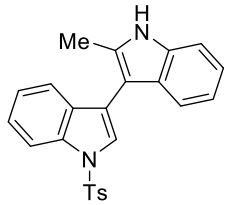


5al

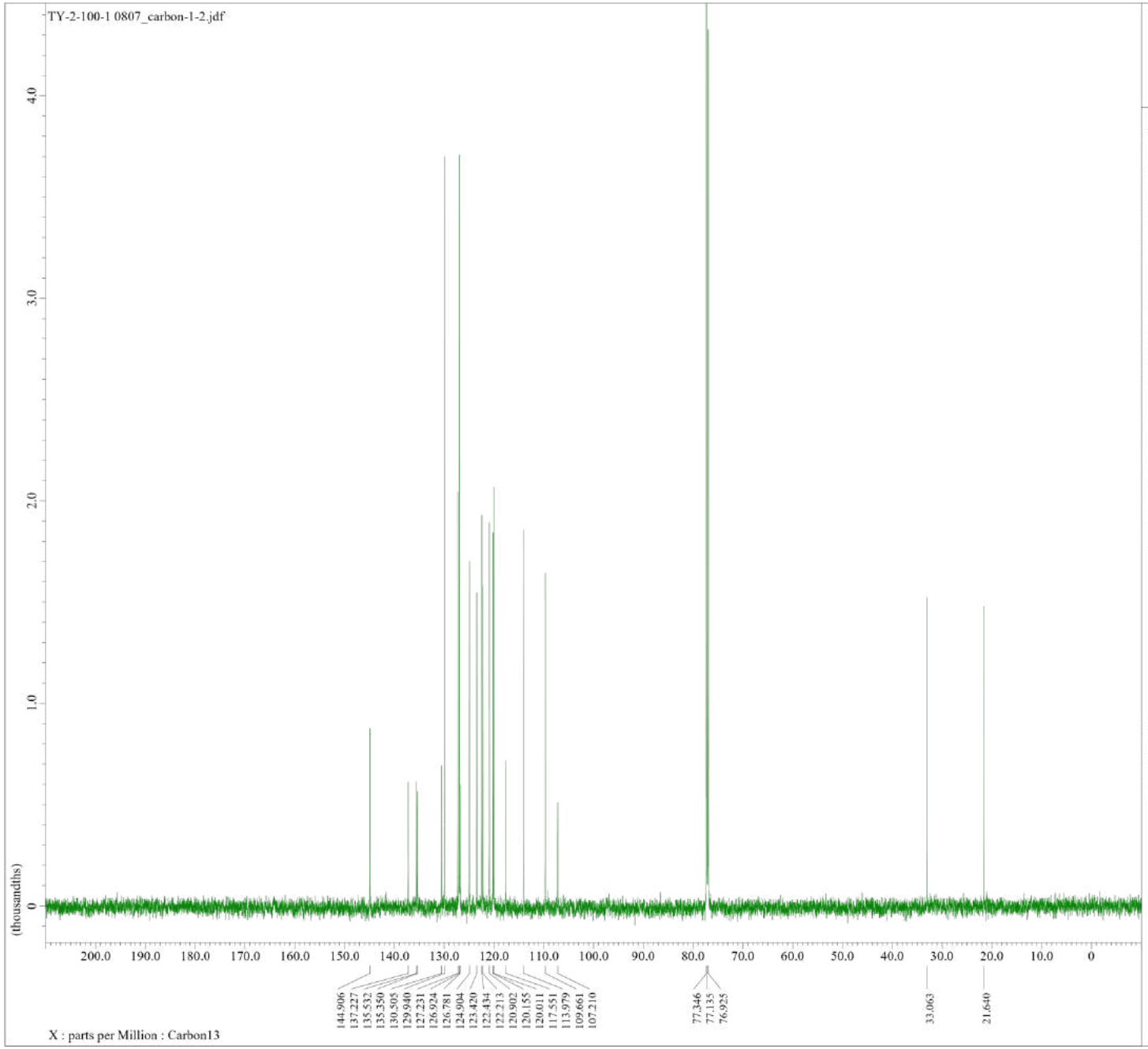


JEOL

Filename	= TY-2-100-1 0807_proto
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-100-1 0807
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-AUG-2021 09:01:10
Revision_Time	= 7-AUG-2021 09:55:50
Comment	= N-Et
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 20.9[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

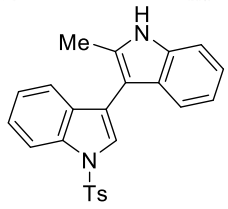


5am

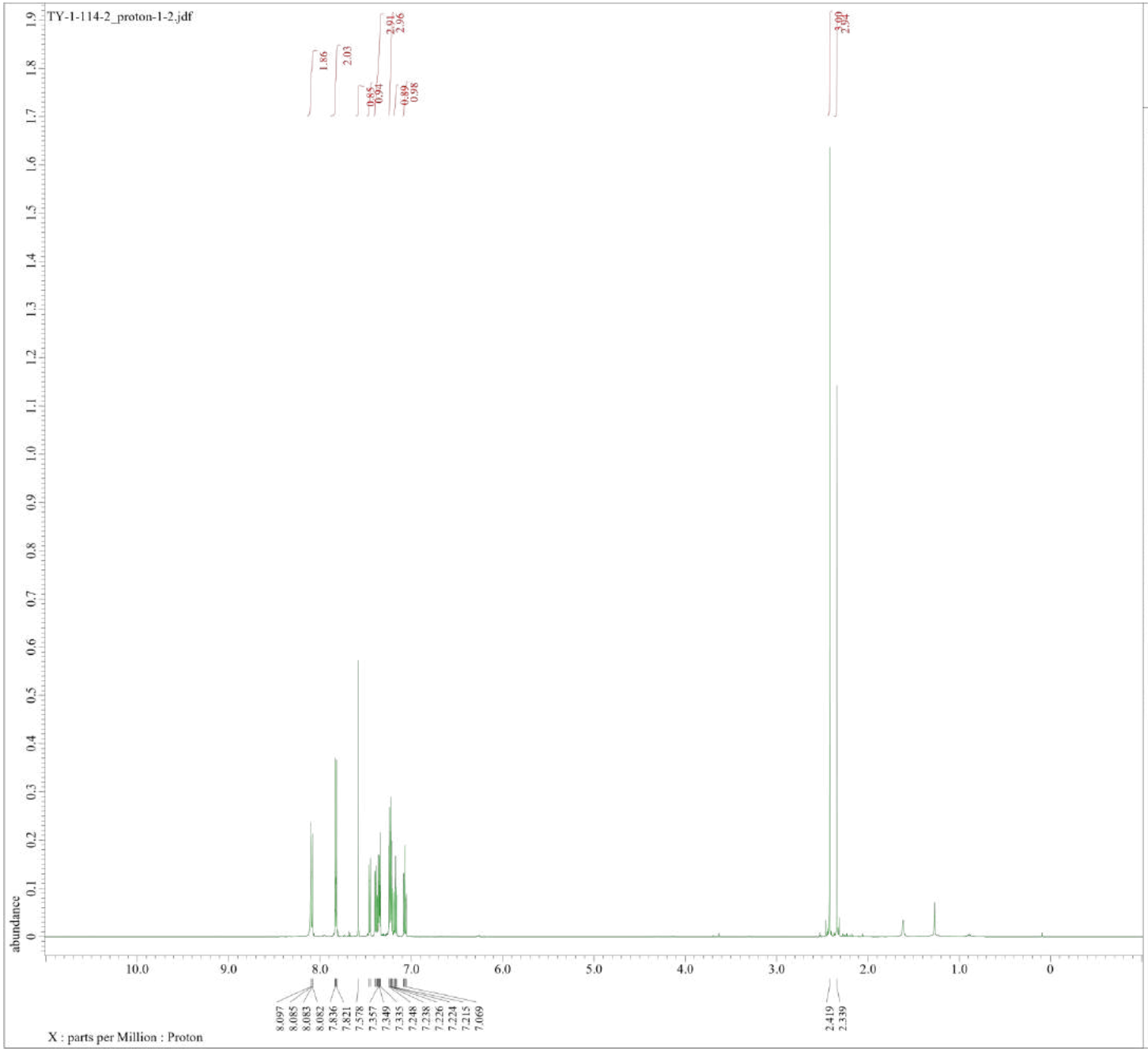


JEOL

Filename	= TY-2-100-1 0807_ca
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-100-1 0807
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-AUG-2021 09:13:
Revision_Time	= 7-AUG-2021 09:57:
Comment	= N-Ms
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 279
Total_Scans	= 279
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 21.2[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]

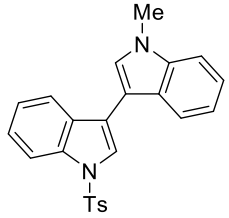


5am

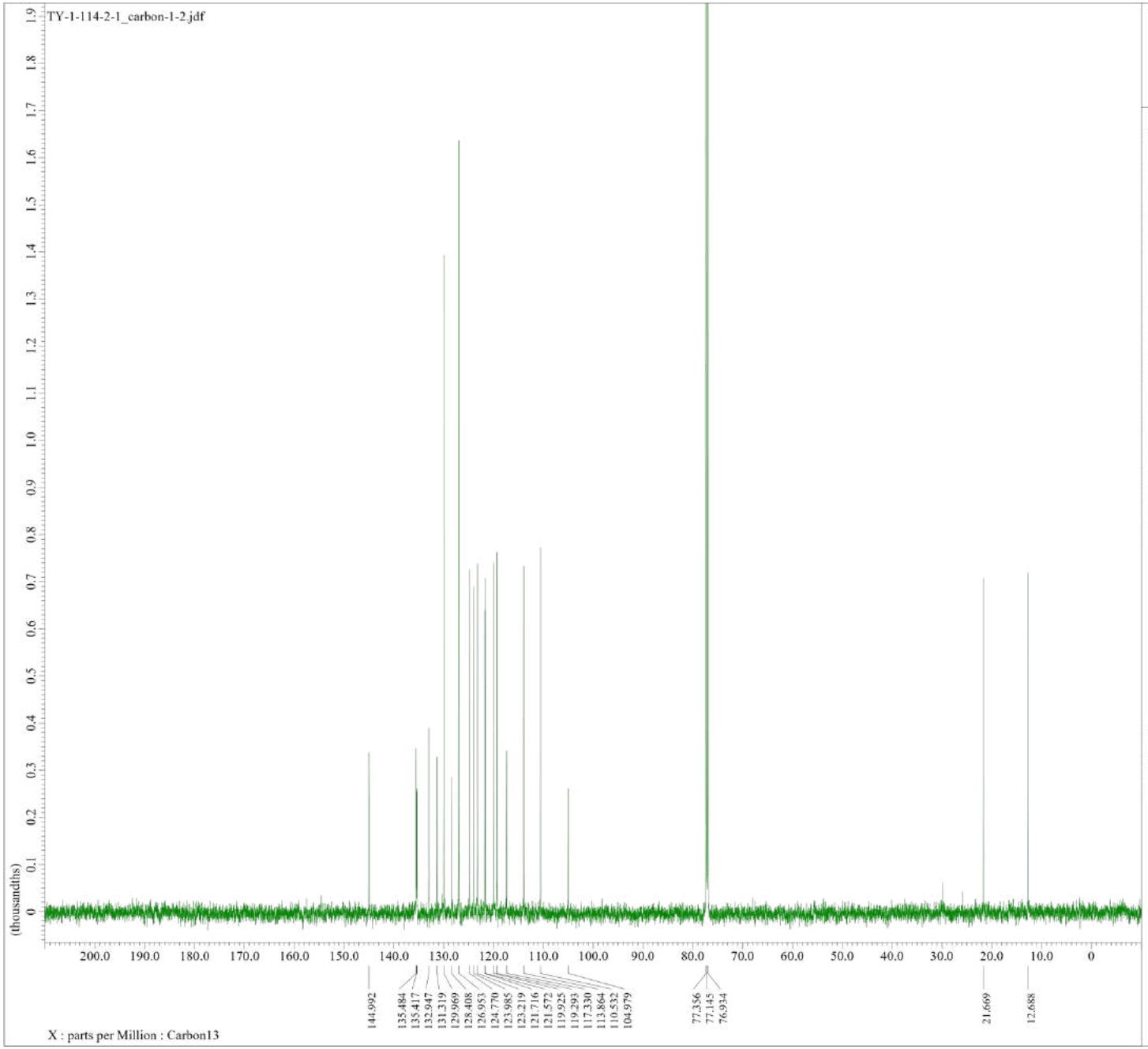


JEOL

Filename	= TY-1-114-2_proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-1-114-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-JUN-2021 11:22:49
Revision_Time	= 7-JUN-2021 12:48:46
Comment	= AZ3
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 20.7[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]

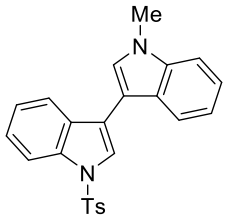


5an



JEOL

Filename	= TY-1-114-2-1_carbo
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-1-114-2-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUN-2021 18:33:
Revision_Time	= 8-JUN-2021 18:45:
Comment	= AZIN 3 2-MeIN
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 201
Total_Scans	= 201
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
Temp_Get	= 20.9[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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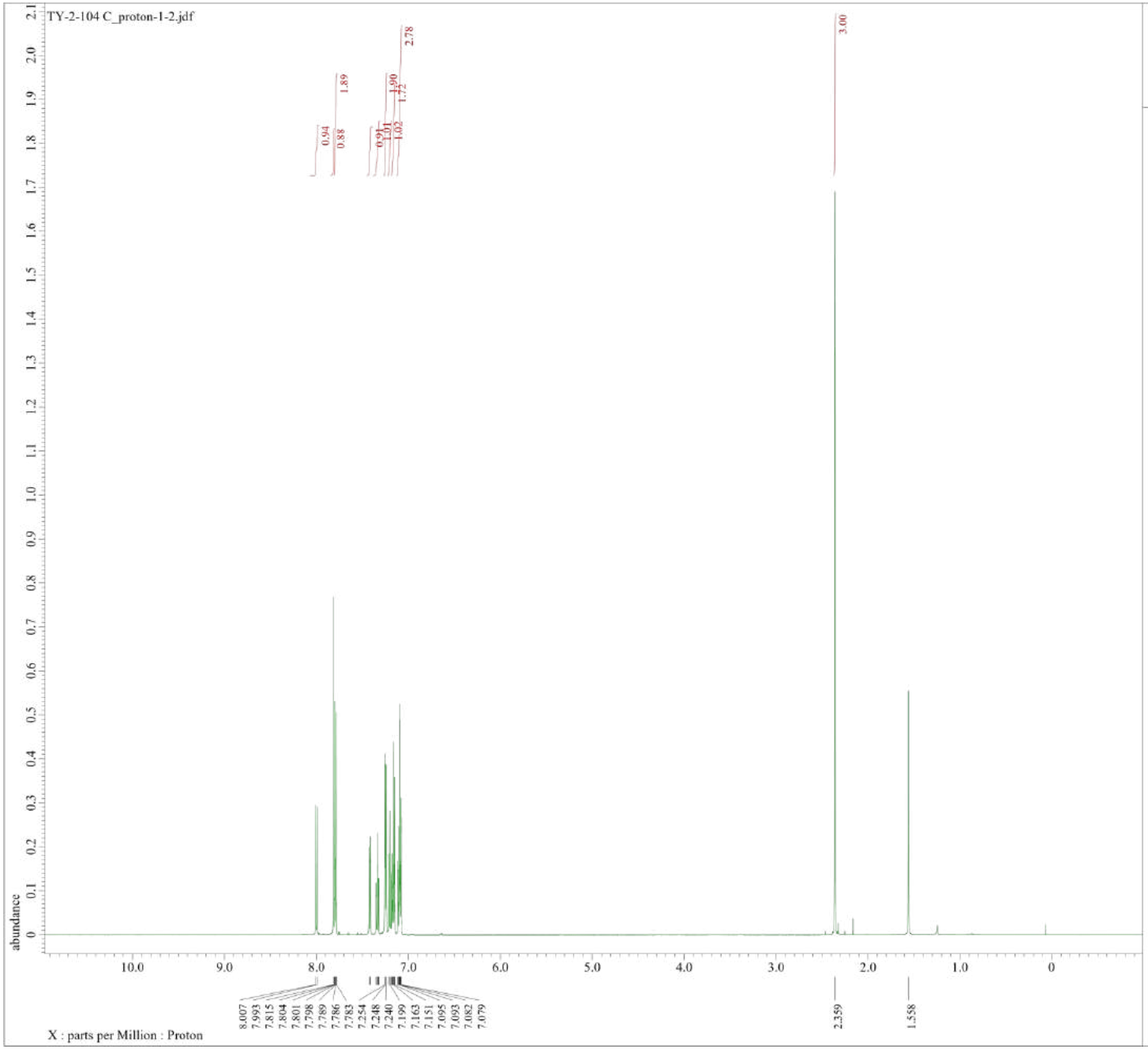
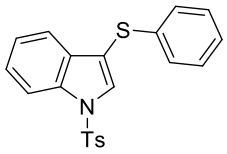


JEOL

Filename	= TY-2-104 C_proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TY-2-104 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-SEP-2021 20:23:51
Revision_Time	= 26-SEP-2021 20:34:29
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.18103808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 46
Temp_Get	= 20.9[dC]
X_90_Width	= 7.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 3.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 100
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 1[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 3.18103808[s]



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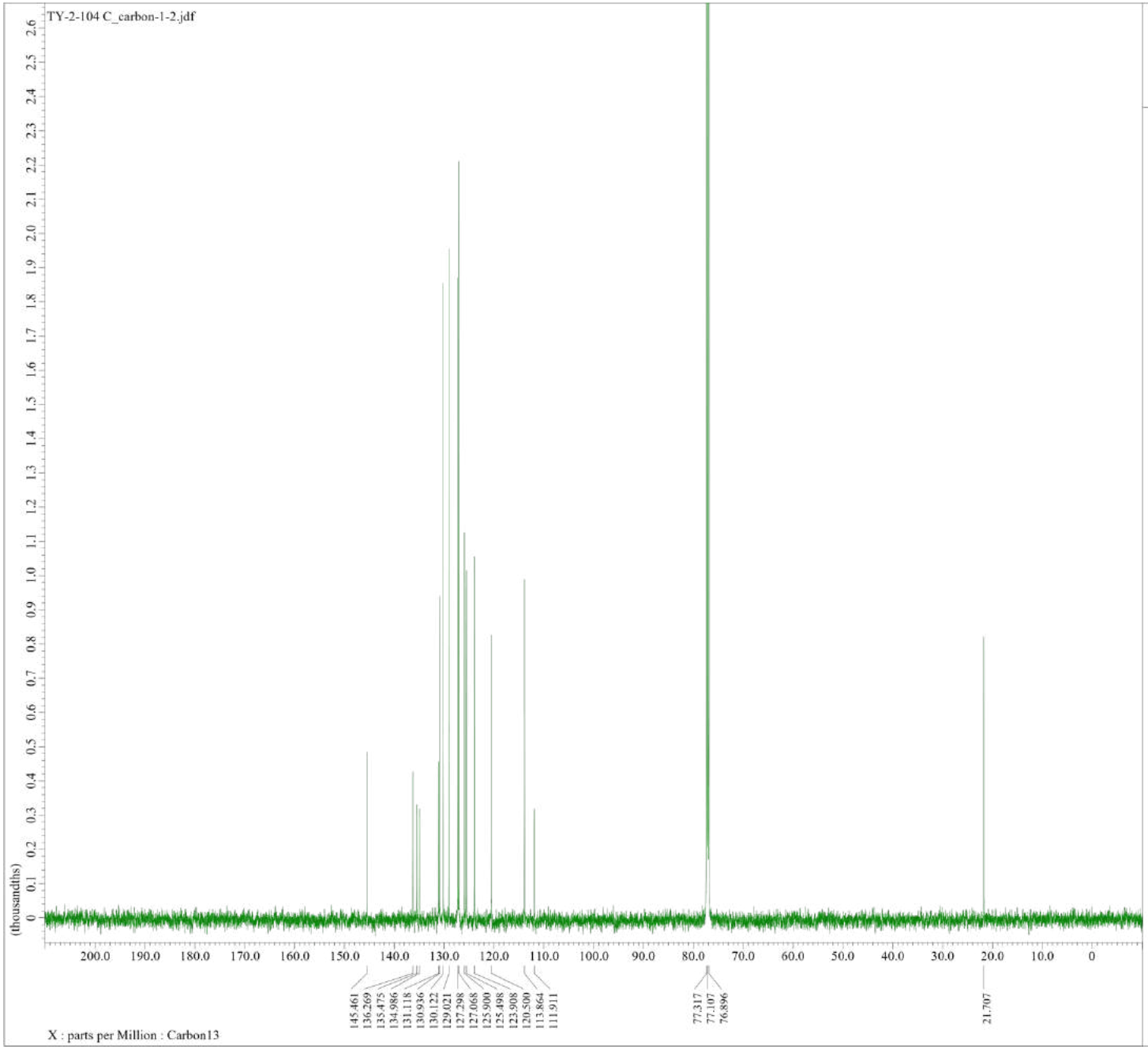
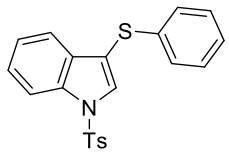


JEOL

Filename	= TY-2-104 C_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-104 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-SEP-2021 20:40:
Revision_Time	= 27-SEP-2021 10:35:
Comment	= SH
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21.6[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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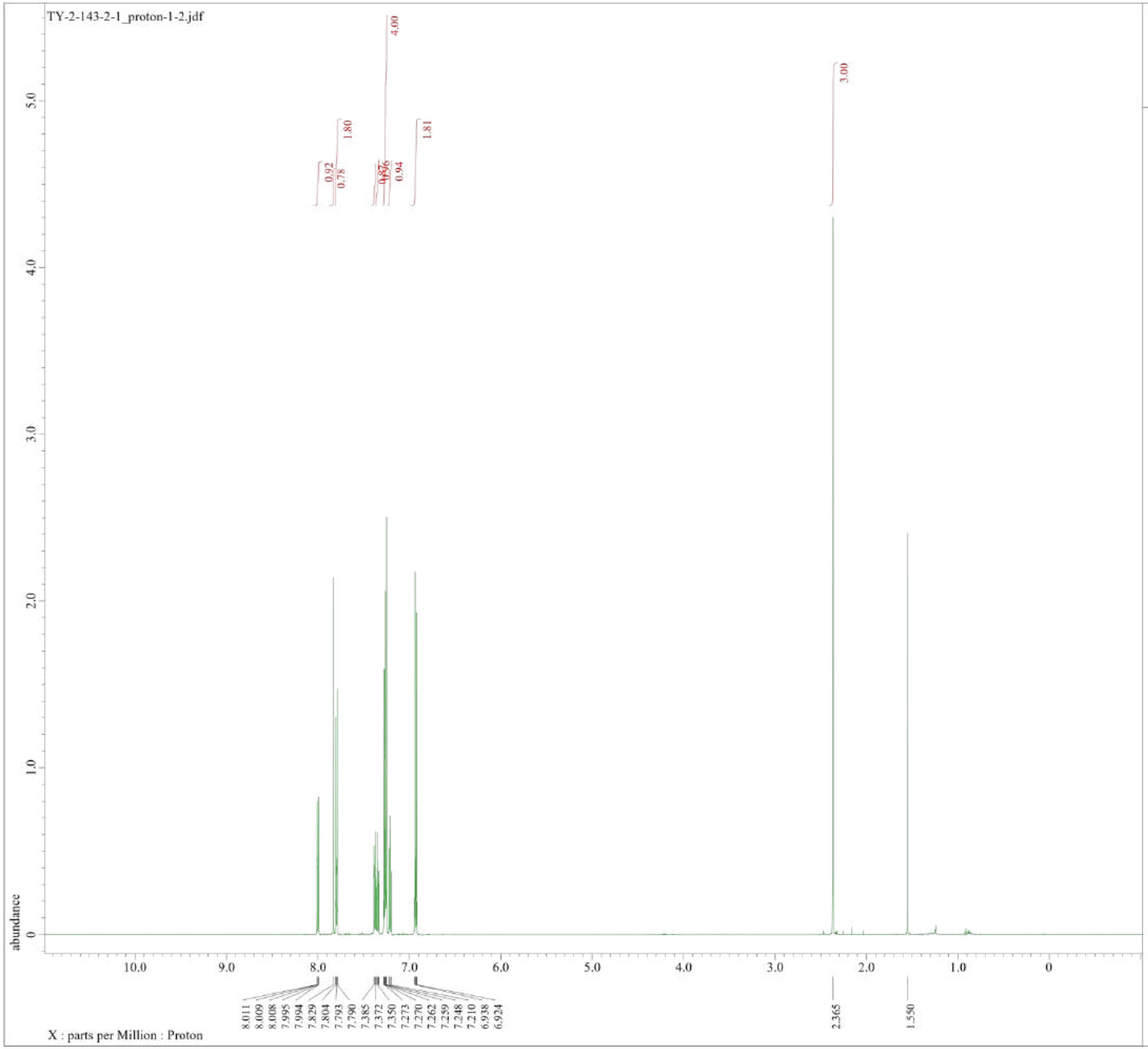
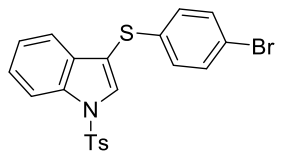



```
Filename              = TY-2-143-2-1_proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-2-143-2-1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 19-SEP-2021 17:18:54
Revision_Time         = 19-SEP-2021 18:22:01

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

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 20.8[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = (0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



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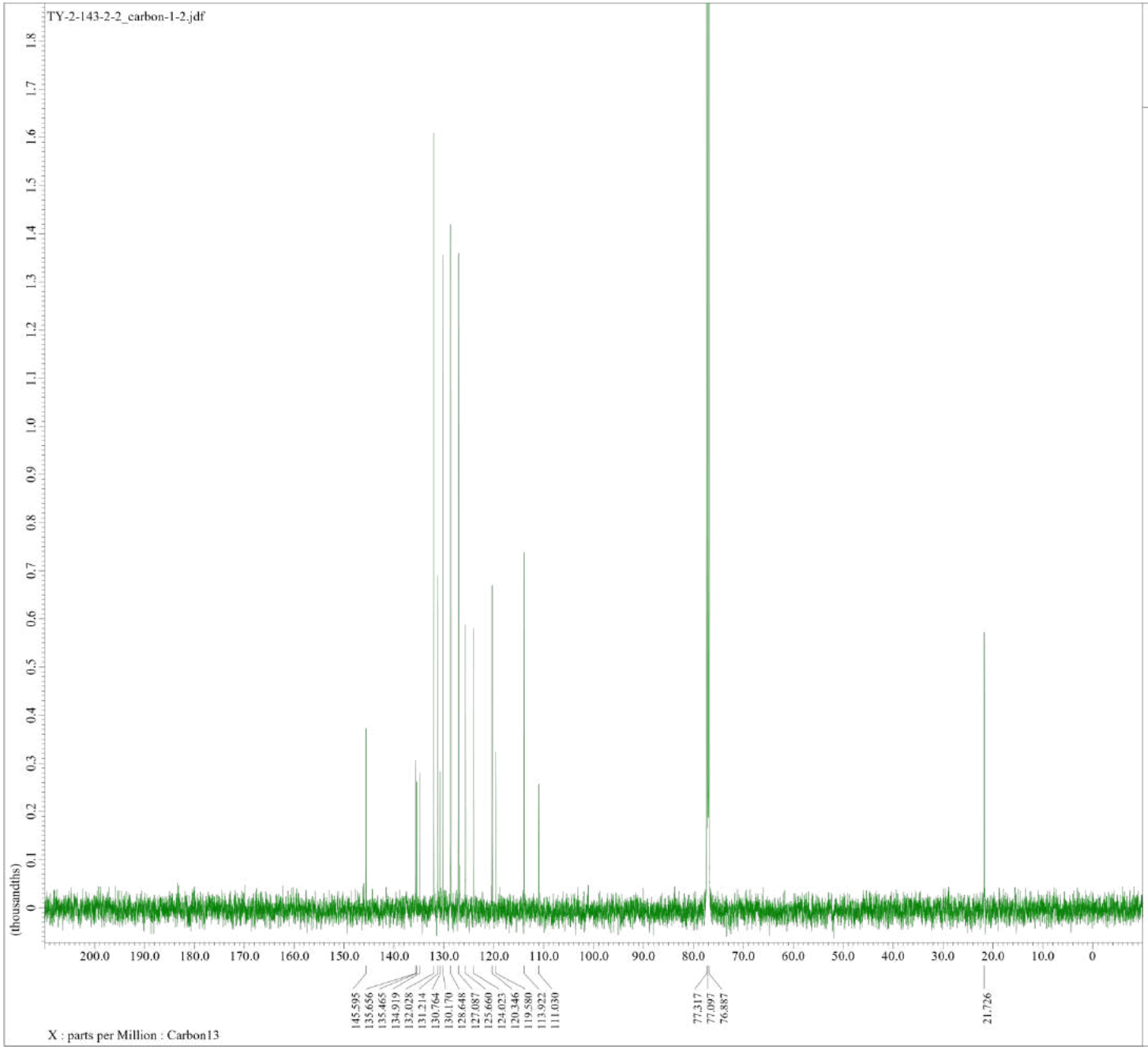
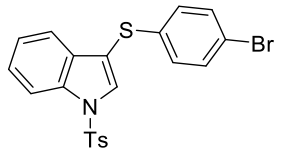


JEOL

Filename	= TY-2-143-2-2_carbo
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-143-2-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-SEP-2021 17:45:
Revision_Time	= 19-SEP-2021 18:05:
Comment	= 4BrSH
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 534
Total_Scans	= 534
Relaxation_Delay	= 2[s]
Recvr_Gain	= 36
Temp_Get	= 21.1[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.6[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 27.986[dB]
Irr_Atn_Dec_Calc	= 27.986[dB]
Irr_Atn_Dec_Default_Calc	= 27.986[dB]
Irr_Atn_Noe	= 27.986[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
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]



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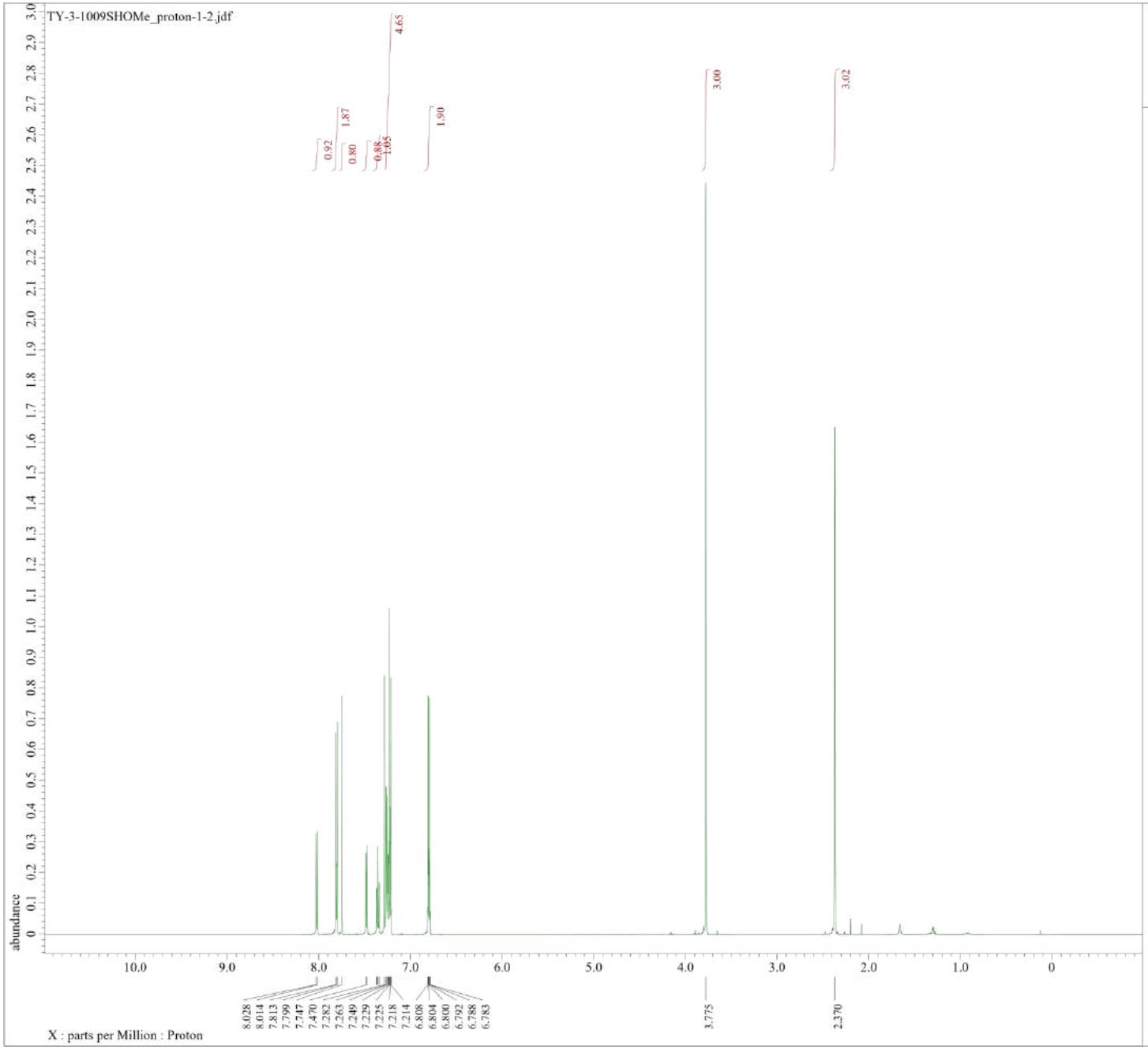


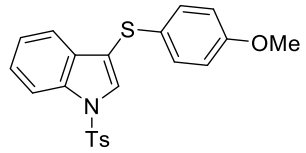
JEOL

```
Filename              = TY-3-1009SHOMe_proton
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-3-1009SHOMe
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  9-OCT-2021 14:13:52
Revision_Time         =  9-OCT-2021 14:09:31

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

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 5[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 26
Temp_Get              = 20.9[dC]
X_90_Width            = 9.4[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 4.7[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



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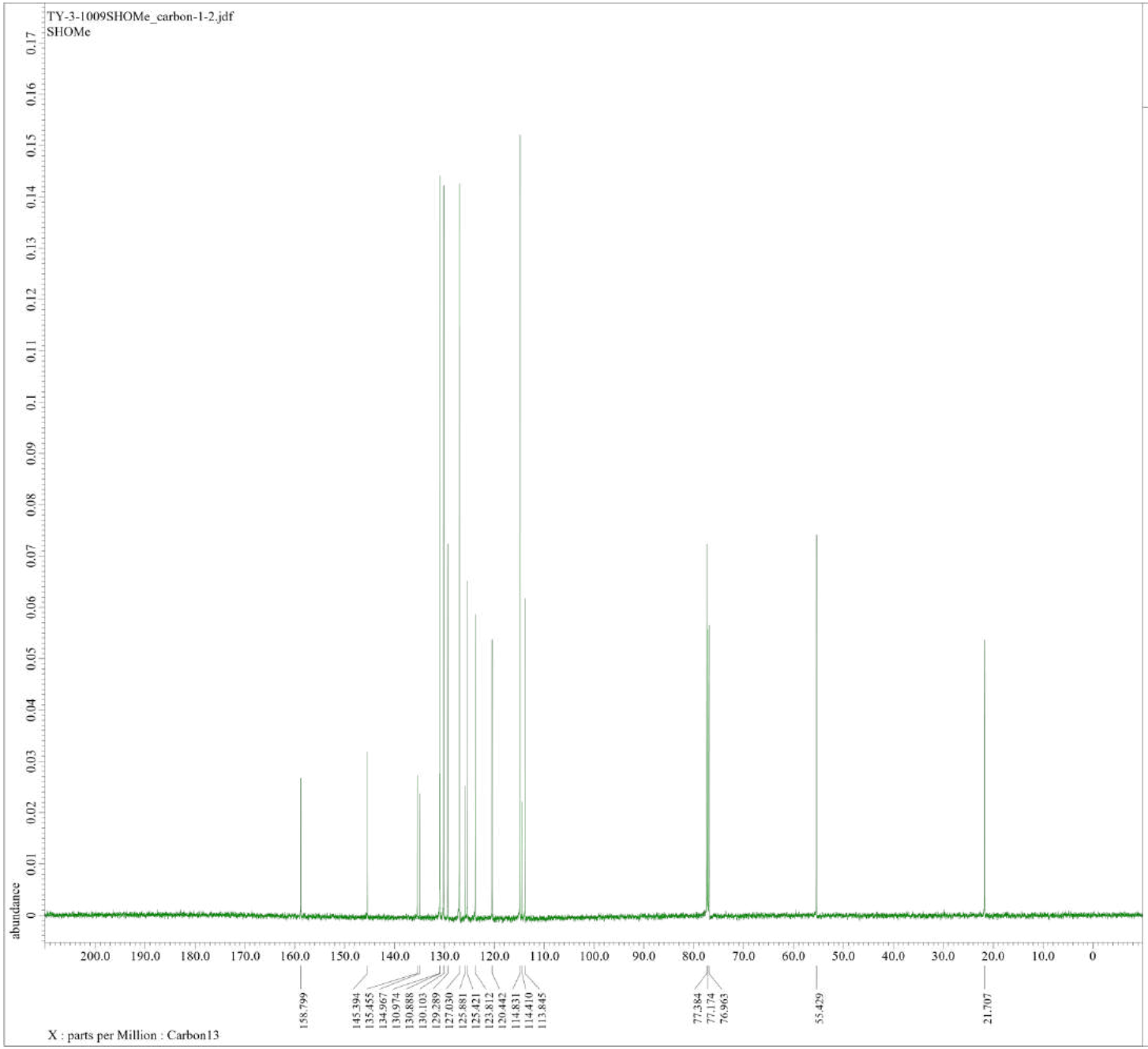
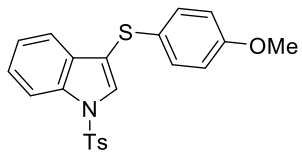
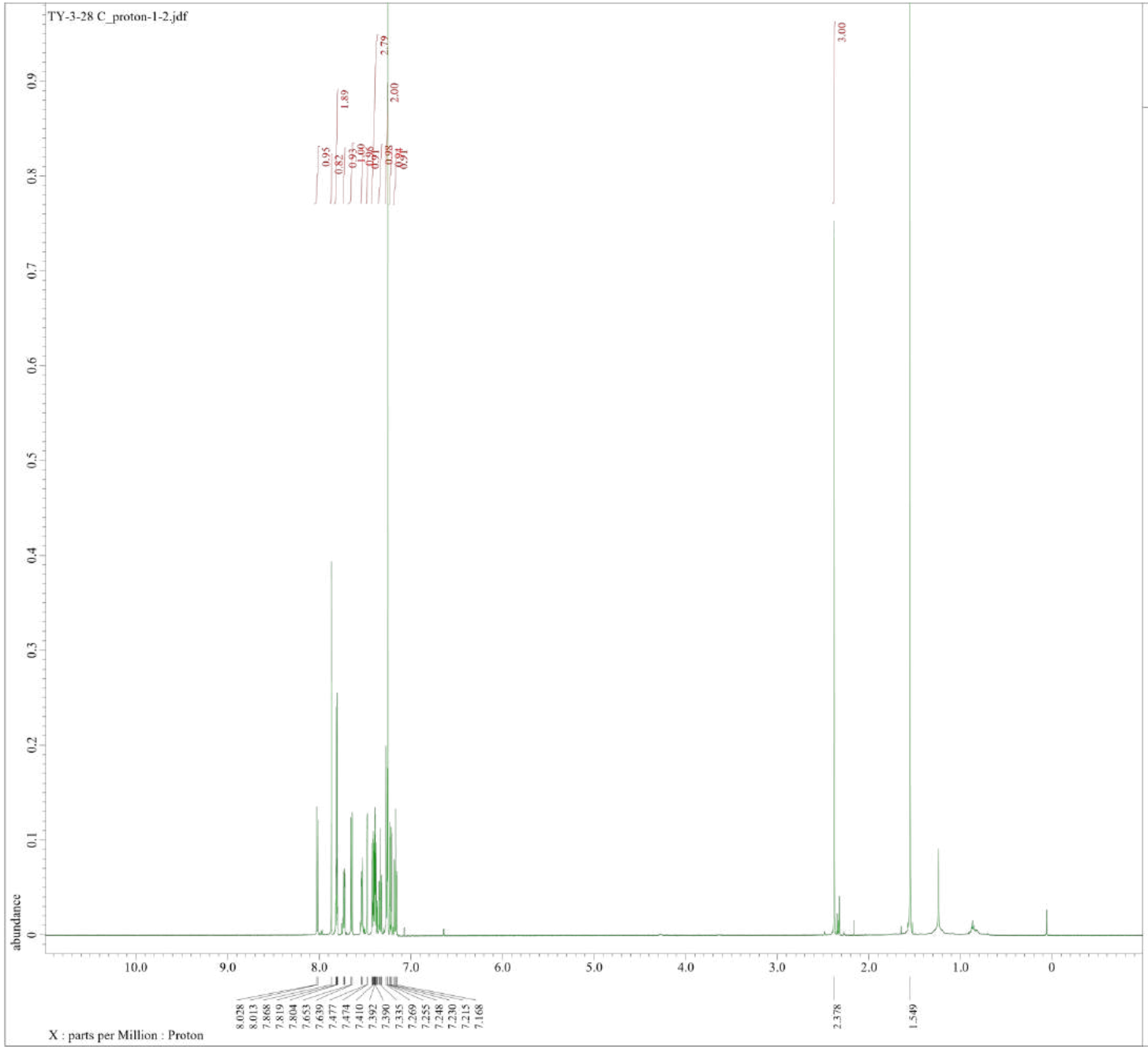


JEOL

Filename	= TY-3-1009SHOMe_car
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-3-1009SHOMe
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-OCT-2021 14:17:
Revision_Time	= 9-OCT-2021 14:12:
Comment	= SHOMe
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15[us]
Clipped	= FALSE
Scans	= 47
Total_Scans	= 47
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21[dC]
X_90_Width	= 9.6[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 3.2[us]
Irr_Atn_Dec	= 26.254[dB]
Irr_Atn_Dec_Calc	= 26.254[dB]
Irr_Atn_Dec_Default_Calc	= 26.254[dB]
Irr_Atn_Noe	= 26.254[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



5aq



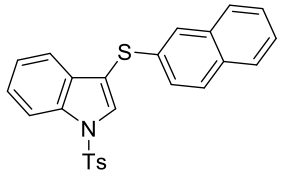
JEOL

```
Filename              = TY-3-28 C_proton-1-2.
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TY-3-28 C
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 26-SEP-2021 20:28:25
Revision_Time         = 26-SEP-2021 20:45:42

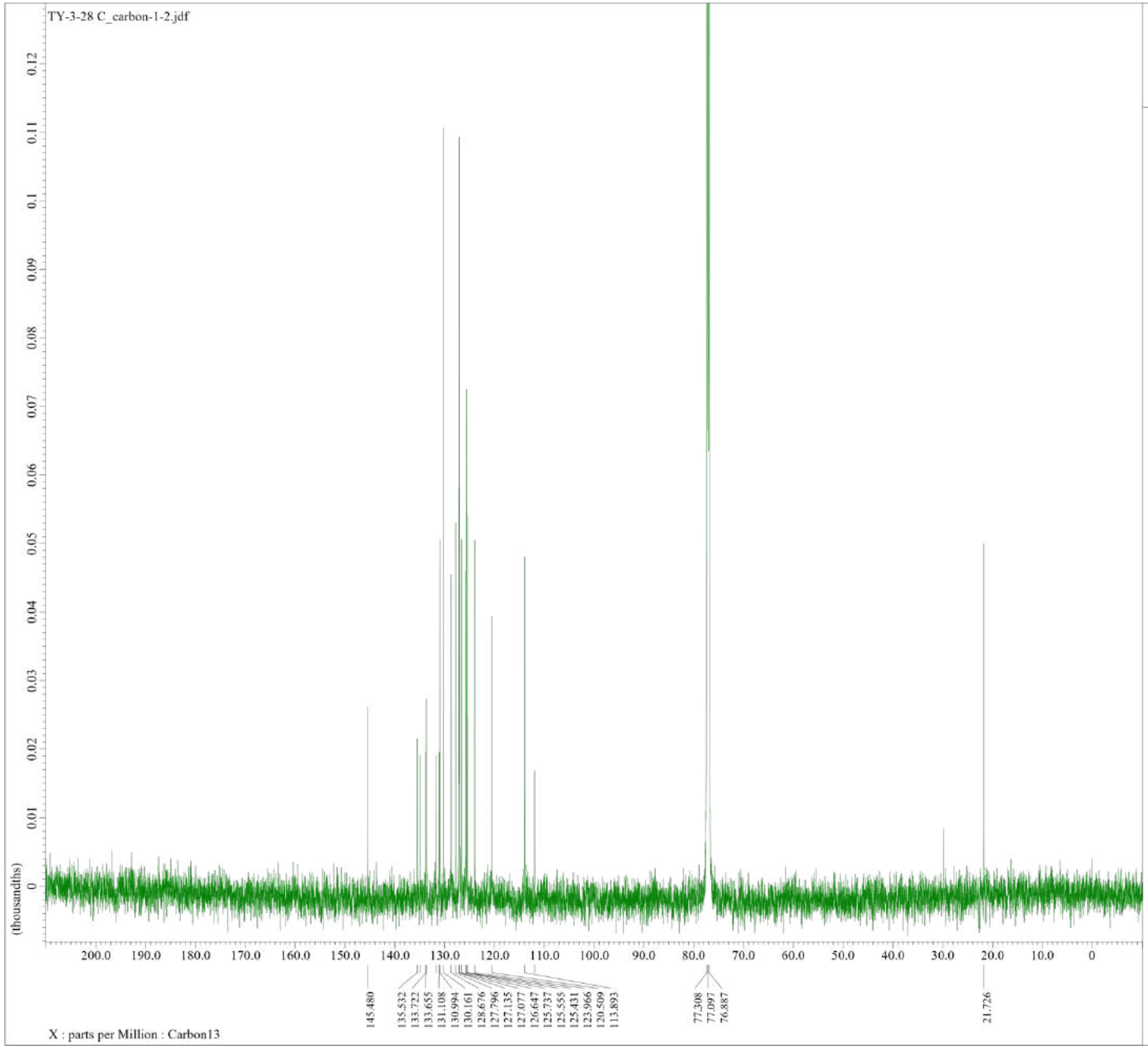
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 2.18103808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 32768
X_Prescans            = 1
X_Resolution          = 0.45849727[Hz]
X_Sweep               = 15.02403846[kHz]
X_Sweep_Clipped       = 12.01923077[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 1[s]
Recvr_Gain            = 56
Temp_Get              = 20.9[dC]
X_90_Width            = 7.7[us]
X_Acq_Time            = 2.18103808[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 3.85[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 100
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JEOL
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180
Presat_Time           = 1[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]
Repetition_Time       = 3.18103808[s]
```



5ar

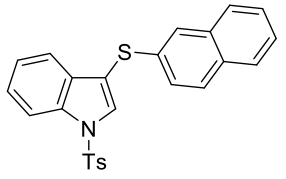



```
Filename                = TY-3-28 C_carbon-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = TY-3-28 C
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 26-SEP-2021 21:30:
Revision_Time           = 27-SEP-2021 10:33:

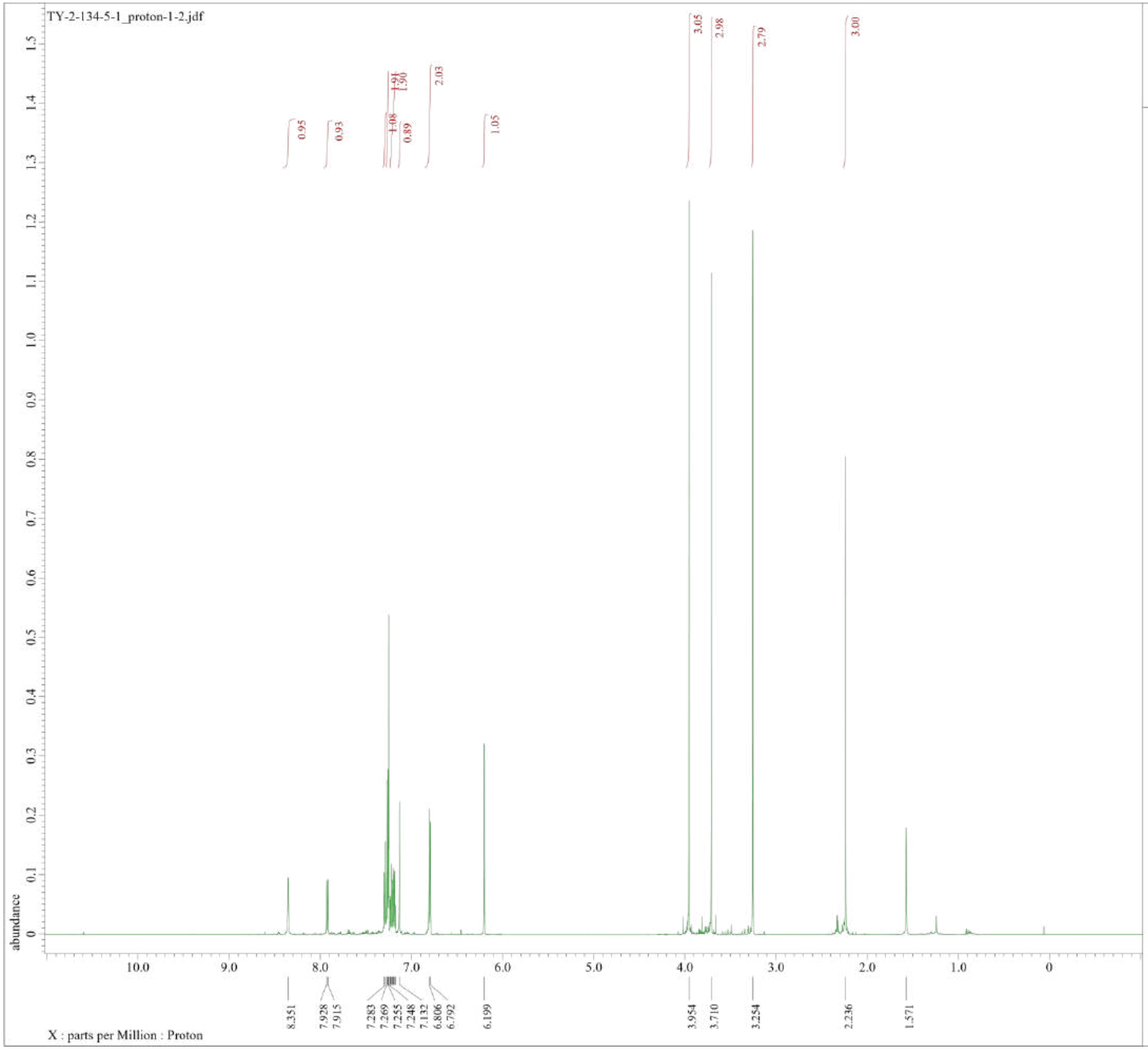
Comment                 = SH naph
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (60
X_Acq_Duration          = 0.69206016[s]
X_Domain                = Carbon13
X_Freq                  = 150.91343039[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 1.44496109[Hz]
X_Sweep                 = 47.34848485[kHz]
X_Sweep_Clipped         = 37.87878788[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8192
Total_Scans             = 8192

Relaxation_Delay        = 2[s]
Recvr_Gain              = 26
Temp_Get                = 21.1[dC]
X_90_Width              = 11.8[us]
X_Acq_Time              = 0.69206016[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.6[dB]
X_Pulse                 = 3.93333333[us]
Irr_Atn_Dec             = 27.986[dB]
Irr_Atn_Dec_Calc        = 27.986[dB]
Irr_Atn_Dec_Default_Calc = 27.986[dB]
Irr_Atn_Noe             = 27.986[dB]
Irr_Dec_Bandwidth_Hz    = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm   = 12.05794078[ppm]
Irr_Dec_Freq            = 600.1723046[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 76[us]
Irr_Pwidth_Default      = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1        = 76[us]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
Experiment_Path         = c:\Program Files\J
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]
```



5ar



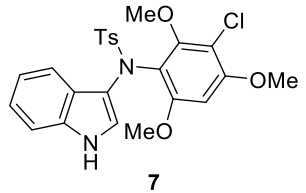
JEOL

```
Filename                = TY-2-134-5-1_proton-1
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TY-2-134-5-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 18-OCT-2021 21:27:12
Revision_Time           = 18-OCT-2021 21:22:52

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

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 2.18103808[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 32768
X_Prescans              = 1
X_Resolution            = 0.45849727[Hz]
X_Sweep                 = 15.02403846[kHz]
X_Sweep_Clipped         = 12.01923077[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 1[s]
Recvr_Gain              = 36
Temp_Get                = 20.3[dC]
X_90_Width              = 9.4[us]
X_Acq_Time              = 2.18103808[s]
X_Angle                 = 45[deg]
X_Atn                   = 8.1[dB]
X_Pulse                 = 4.7[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 100
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = c:\Program Files\JEOL
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 1[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 1[s]
Repetition_Time         = 3.18103808[s]
```



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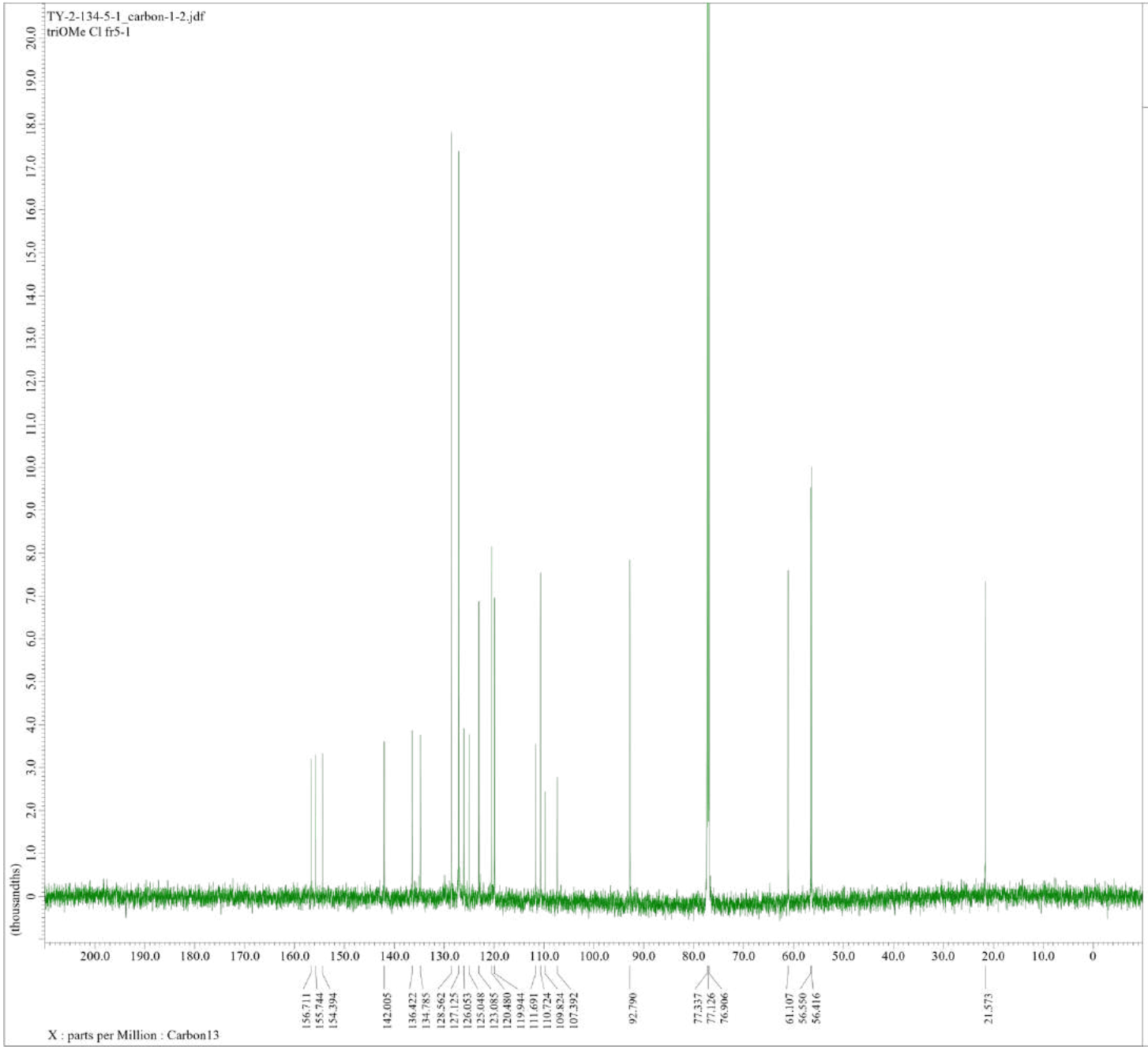
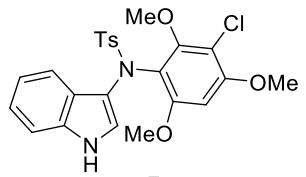
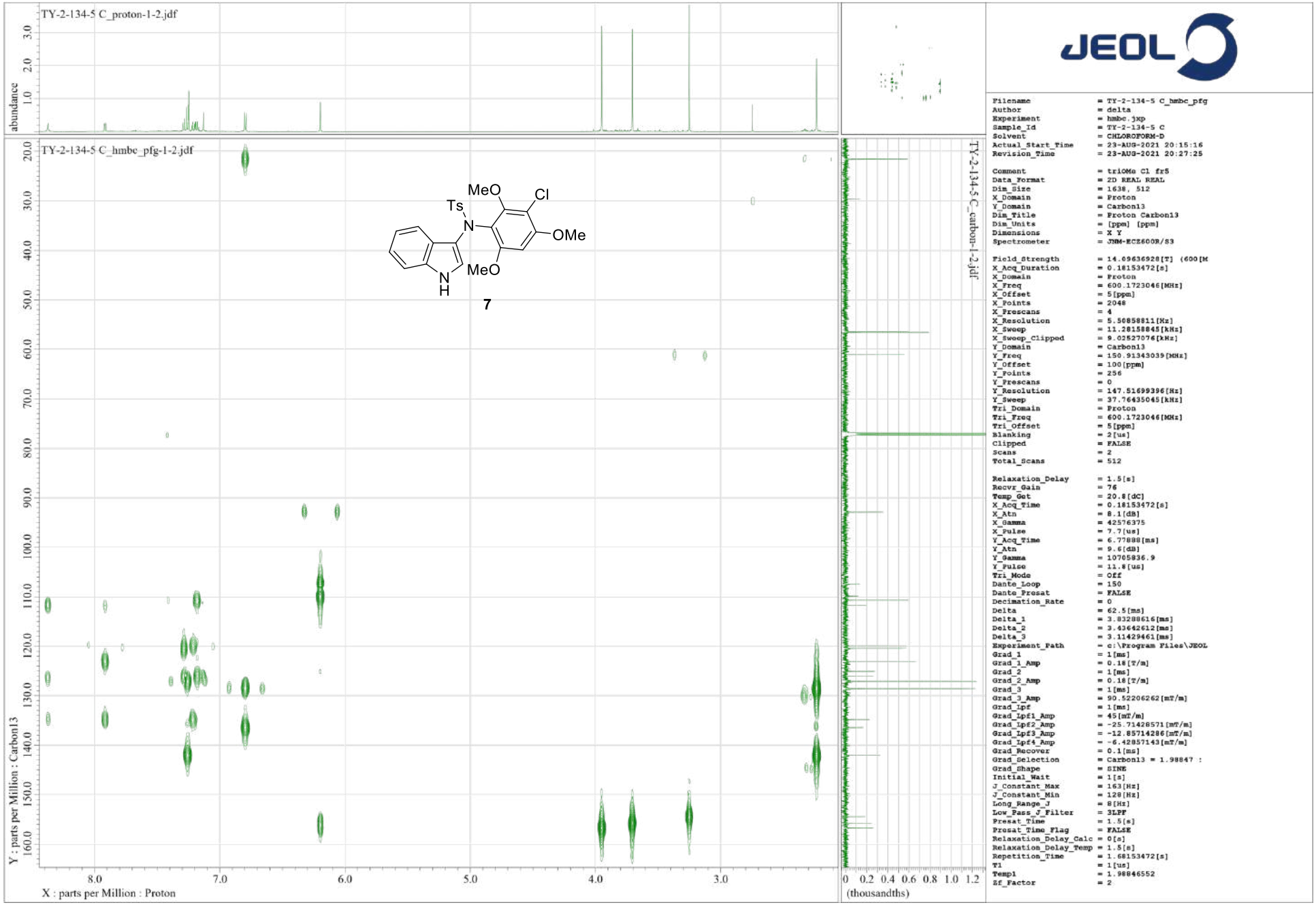


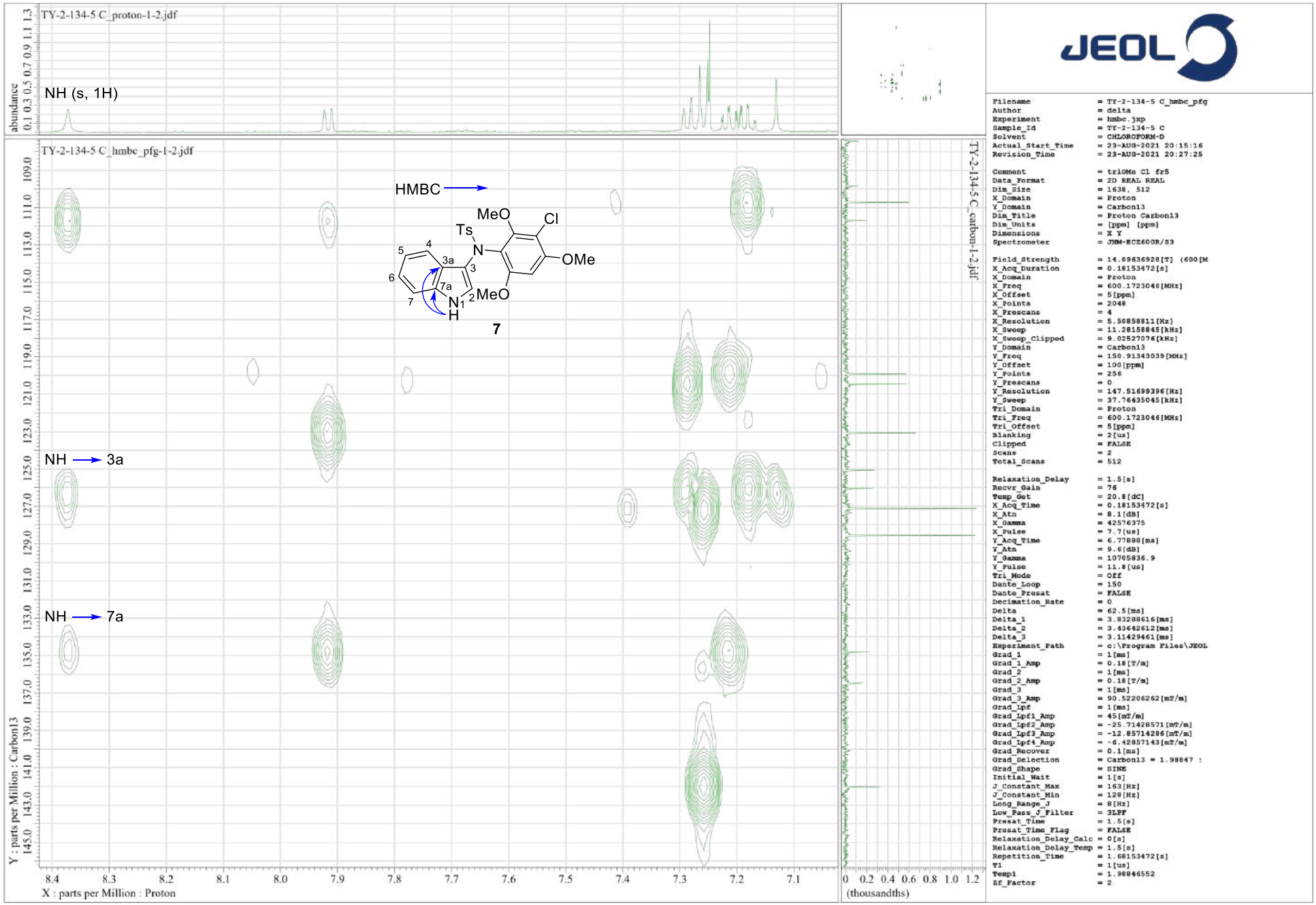
JEOL

Filename	= TY-2-134-5-1_carbo
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TY-2-134-5-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-OCT-2021 21:28:
Revision_Time	= 18-OCT-2021 21:31:
Comment	= triOMe Cl fr5-1
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 15[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20[dC]
X_90_Width	= 9.6[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 3.2[us]
Irr_Atn_Dec	= 26.254[dB]
Irr_Atn_Dec_Calc	= 26.254[dB]
Irr_Atn_Dec_Default_Calc	= 26.254[dB]
Irr_Atn_Noe	= 26.254[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]
Repetition_Time	= 1.69206016[s]



7


TY-2-134-5 C_proton-1-2.jdf
abundance
TY-2-134-5 C_hmbc_pfg-1-2.jdf
MeO
Cl
Ts
N
OMe
MeO
N
H
7
TY-2-134-5 C_carbon-1-2.jdf
Y : parts per Million : Carbon13
X : parts per Million : Proton
(thousandths)
Filename = TY-2-134-5 C_hmbc_pfg
Author = delta
Experiment = hmbc.jxp
Sample_Id = TY-2-134-5 C
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-AUG-2021 20:15:16
Revision_Time = 23-AUG-2021 20:27:25
Comment = triOMe Cl fr5
Data_Format = 2D REAL REAL
Dim_Size = 1638, 512
X_Domain = Proton
Y_Domain = Carbon13
Dim_Title = Proton Carbon13
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.18153472[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 5.50858811[Hz]
X_Sweep = 11.28158845[kHz]
X_Sweep_Clipped = 9.02527076[kHz]
Y_Domain = Carbon13
Y_Freq = 150.91343039[MHz]
Y_Offset = 100[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 147.51699396[Hz]
Y_Sweep = 37.76435045[kHz]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 2
Total_Scans = 512
Relaxation_Delay = 1.5[s]
Recvr_Gain = 76
Temp_Get = 20.8[dC]
X_Acq_Time = 0.18153472[s]
X_Atn = 8.1[dB]
X_Gamma = 42576375
X_Pulse = 7.7[us]
Y_Acq_Time = 6.77888[ms]
Y_Atn = 9.6[dB]
Y_Gamma = 10705836.9
Y_Pulse = 11.8[us]
Tri_Mode = Off
Dante_Loop = 150
Dante_Presat = FALSE
Decimation_Rate = 0
Delta = 62.5[ms]
Delta_1 = 3.83288616[ms]
Delta_2 = 3.43642612[ms]
Delta_3 = 3.11429461[ms]
Experiment_Path = c:\Program Files\JEOL
Grad_1 = 1[ms]
Grad_1_Amp = 0.18[T/m]
Grad_2 = 1[ms]
Grad_2_Amp = 0.18[T/m]
Grad_3 = 1[ms]
Grad_3_Amp = 90.52206262[mT/m]
Grad_lpf = 1[ms]
Grad_lpf1_Amp = 45[mT/m]
Grad_lpf2_Amp = -25.71428571[mT/m]
Grad_lpf3_Amp = -12.85714286[mT/m]
Grad_lpf4_Amp = -6.42857143[mT/m]
Grad_Recover = 0.1[ms]
Grad_Selection = Carbon13 = 1.98847 :
Grad_Shape = SINE
Initial_Wait = 1[s]
J_Constant_Max = 163[Hz]
J_Constant_Min = 129[Hz]
Long_Range_J = 8[Hz]
Low_Pass_J_Filter = 3LPF
Presat_Time = 1.5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1.5[s]
Repetition_Time = 1.68153472[s]
T1 = 1[us]
Temp1 = 1.98846552
Zf_Factor = 2



JEOL

Filename	= TY-2-134-5 C_hmbc_pfg
Author	= delta
Experiment	= hmbc.jxp
Sample_Id	= TY-2-134-5 C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-AUG-2021 20:15:16
Revision_Time	= 23-AUG-2021 20:27:25
Comment	= triOMe Cl fr5
Data_Format	= 2D REAL REAL
Dim_Size	= 1638, 512
X_Domain	= Proton
Y_Domain	= Carbon13
Dim_Title	= Proton Carbon13
Dim_Units	= [ppm] [ppm]
Dimensions	= X Y
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.18153472[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 2048
X_Prescans	= 4
X_Resolution	= 5.50858811[Hz]
X_Sweep	= 11.28158845[kHz]
X_Sweep_Clipped	= 9.02527076[kHz]
Y_Domain	= Carbon13
Y_Freq	= 150.91343039[MHz]
Y_Offset	= 100[ppm]
Y_Points	= 256
Y_Prescans	= 0
Y_Resolution	= 147.51699396[Hz]
Y_Sweep	= 37.76435045[kHz]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 2
Total_Scans	= 512
Relaxation_Delay	= 1.5[s]
Recvr_Gain	= 76
Temp_Get	= 20.8[dC]
X_Acq_Time	= 0.18153472[s]
X_Atn	= 8.1[dB]
X_Gamma	= 42576375
X_Pulse	= 7.7[us]
Y_Acq_Time	= 6.77888[ms]
Y_Atn	= 9.6[dB]
Y_Gamma	= 10705836.9
Y_Pulse	= 11.8[us]
Tri_Mode	= Off
Dante_Loop	= 150
Dante_Presat	= FALSE
Decimation_Rate	= 0
Delta	= 62.5[ms]
Delta_1	= 3.83288616[ms]
Delta_2	= 3.43642612[ms]
Delta_3	= 3.11429461[ms]
Experiment_Path	= c:\Program Files\JEOL
Grad_1	= 1[ms]
Grad_1_Amp	= 0.18[T/m]
Grad_2	= 1[ms]
Grad_2_Amp	= 0.18[T/m]
Grad_3	= 1[ms]
Grad_3_Amp	= 90.52206262[mT/m]
Grad_lpf	= 1[ms]
Grad_lpf1_Amp	= 45[mT/m]
Grad_lpf2_Amp	= -25.71428571[mT/m]
Grad_lpf3_Amp	= -12.85714286[mT/m]
Grad_lpf4_Amp	= -6.42857143[mT/m]
Grad_Recover	= 0.1[ms]
Grad_Selection	= Carbon13 = 1.98847 :
Grad_Shape	= SINE
Initial_Wait	= 1[s]
J_Constant_Max	= 163[Hz]
J_Constant_Min	= 128[Hz]
Long_Range_J	= 8[Hz]
Low_Pass_J_Filter	= 3LPF
Presat_Time	= 1.5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1.5[s]
Repetition_Time	= 1.68153472[s]
T1	= 1[us]
Temp1	= 1.98846552
Zf_Factor	= 2

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