Electronic Supplementary Material (ESI) for ChemComm.

Synthesis of α-Substituted Indolylacetamide using Acetonitriles as Acetamide Enolate Equivalents through *O*-Transfer Reactions

Takumi Abe*, Kenta Noda, and Daisuke Sawada*
Graduate School of Medicine, Dentistry and Pharmaceutical Sciences, Okayama University, 1-1-1 Tsushima-naka,
Kita-ku, Okayama 7008530, Japan
E-mail: t-abe@okayama-u.ac.jp
dsawada@okayama-u.ac.jp

SUPPORTING INFORMATION

Contents

Experimental Section

Mass-spectrometry

High-resolution mass spectra were recorded with a Brucker micrOTOF mass spectrometers (ESI-TOF-MS).

NMR spectroscopy

NMR experiments were performed with a JEOL JNM-ECX600 spectrometer operating at 600 MHz and 151 MHz for ^{1}H and ^{13}C acquisitions, respectively. Chemical shifts are expressed in ppm (δ) using residual solvent as the internal reference. For ^{1}H NMR: $CDCl_3$, δ 7.25; DMSO-d_6, δ 2.50; acetone-d_6, δ 2.02; For ^{13}C NMR: $CDCl_3$, δ 77.1; DMSO-d_6, δ 39.5; acetone-d_6, δ 29.1. NMR peak are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, ddd = doublet of doublet of doublets, td = triplet of doublets, br s= broad singlet; coupling constants in Hz; integration.

Chromatography

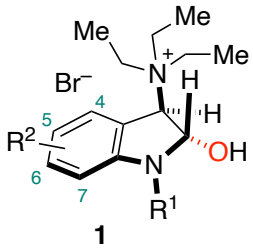
Reactions were monitored by thin layer chromatography (TLC) carried out on a silica gel plates (60F-254) and visualized under UV illumination at 254 or 366 nm depending on the compounds. Column chromatography was performed on silica gel (WAKO Gel 75–150 mesh, WAKO Co., Ltd.).

Starting materials

The HITABs (2-hydroxyindoline-3-triethylammonium bromides, **1**) were prepared by reported methods.[S1-2]

All substrates were used as received from commercial suppliers (Sigma-Aldrich, TCI, and Wako) and all reagents were weighed and handled in air at room temperature.

Synthesis of 2-hydroxyindoline-3-triethylammonium bromides (1)

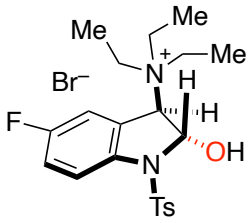


1

1a: R^1 = Ts, R^2 = H
1b: R^1 = Ts, R^2 = 5-MeO
1c: R^1 = Ts, R^2 = 5-Cl
1d: R^1 = Ts, R^2 = 5-Br
1e: R^1 = Ts, R^2 = 5-F

1f: R^1 = Ts, R^2 = 4-F
1g: R^1 = Ts, R^2 = 6-F
1h: R^1 = Ts, R^2 = 7-F
1i: R^1 = Bs, R^2 = H

trans-5-fluoro-2-Hydroxy-1-tosylindoline-3-ammonium bromide (1e)

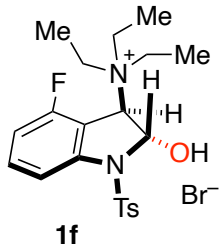


1e

To a solution of 5-fluoro-1-tosylindole (578.7 mg, 2 mmol) and H_2O (0.36 mL, 20 mmol) in acetone (10 mL) was added NBS (355.9 mg, 2.0 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material as indicated by TLC. Et_3N (0.28 mL, 2.0 mmol) was added to the mixture and stirred further 16 h. The resulting precipitate was separated by filtration, washed with acetone, and dried *in vacuo* to give **1e** (707.3 mg, 73% yield).

707.3 mg, 73% yield. colorless solid; mp: 121.6-124.3 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 8.01 (d, J = 8.4 Hz, 2H), 7.45 (dd, J = 1.8, 9.0 Hz, 1H), 7.39 (d, J = 9.0 Hz, 2H), 7.30-7.37 (m, 2H), 6.37 (s, 1H), 4.85 (s, 1H), 3.33–3.48 (m, 6H), 2.33 (s, 3H), 1.00 (t, J = 6.6 Hz, 9H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 180.0, 158.6 (d, $J_{C\text{-}F}$ = 241.5 Hz), 145.5, 139.3, 130.5, 128.2, 122.2 (d, $J_{C\text{-}F}$ = 8.8 Hz), 119.8 (d, $J_{C\text{-}F}$ = 23.1 Hz), 117.8 (d, $J_{C\text{-}F}$ = 23.1 Hz), 114.9 (d, $J_{C\text{-}F}$ = 8.8 Hz), 85.2, 79.8, 75.0, 53.4, 46.1, 30.1, 21.5, 9.3, 8.8; HRMS (ESI) *m/z*: 407.1805 (Calcd for $C_{21}H_{28}FN_2O_3S$ $[M]^+$: 407.1805).

trans-4-fluoro-2-Hydroxy-1-tosylindoline-3-ammonium bromide (1f)



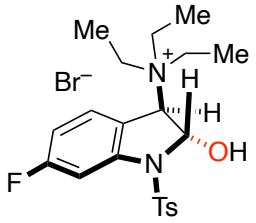
1f

To a solution of 5-fluoro-1-tosylindole (578.7 mg, 2 mmol) and H_2O (0.36 mL, 20 mmol) in acetone (10 mL) was added NBS (355.9 mg, 2.0 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material as indicated by TLC. Et_3N (0.28 mL, 2.0 mmol) was added to the mixture and stirred further 16 h. The resulting precipitate was separated by filtration, washed with acetone, and dried *in vacuo* to give **1e** (483.6 mg,

50% yield).

483.6 mg, 50% yield. colorless solid; mp: 130.6-134.7 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 8.03 (d, J = 9.0 Hz, 2H), 7.54-7.57 (m, 1H), 7.42 (d, J = 8.4 Hz, 2H), 7.02 (t, J = 9.0 Hz, 1H), 6.37 (d, J = 8.4 Hz, 1H), 4.92 (s, 1H), 3.33–3.46 (m, 6H), 2.34 (s, 3H), 1.08 (t, J = 7.2 Hz, 9H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 180.0, 160.7 (d, $J_{C\text{-}F}$ = 251.6 Hz), 145.7, 145.2 (d, $J_{C\text{-}F}$ = 5.9 Hz), 136.0 (d, $J_{C\text{-}F}$ = 10.1Hz), 135.8, 130.5, 128.4, 111.7 (d, $J_{C\text{-}F}$ = 23.1 Hz), 110.0, 107.7 (d, $J_{C\text{-}F}$ = 17.4 Hz), 85.7, 79.7, 73.1, 54.0, 46.2, 30.1, 21.6, 9.1, 9.0; HRMS (ESI) *m/z*: 407.1803 (Calcd for $C_{21}H_{28}FN_2O_3S$ $[M]^+$: 407.1805).

trans-6-fluoro-2-Hydroxy-1-tosylindoline-3-ammonium bromide (1g)

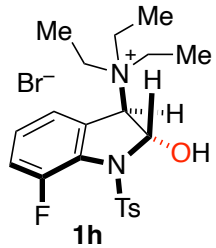


1g

To a solution of 5-fluoro-1-tosylindole (578.7 mg, 2 mmol) and H_2O (0.36 mL, 20 mmol) in acetone (10 mL) was added NBS (355.9 mg, 2.0 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material as indicated by TLC. Et_3N (0.28 mL, 2.0 mmol) was added to the mixture and stirred further 1 h. Then, Et_2O (10 mL) was added to the mixture at 0 °C and stirred further 1h. The resulting precipitate was separated by filtration, washed with acetone/Et_2O (1/1), and dried *in vacuo* to give **1g** (683.9 mg, 70% yield).

683.9 mg, 70% yield. colorless solid; mp: 152.0-155.0 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.93 (m, 2H), 7.48 (m, 1H), 7.20 (m, 2H), 6.96 (m, 1H), 6.64 (m, 1H), 6.53-6.54 (m, 1H), 4.99-5.00 (m, 1H), 3.44–3.47 (m, 6H), 2.25, 2.26, 2.27 (3s, 3H), 1.17-1.29 (m, 9H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 178.6, 178.5, 165.3 (d, $J_{C\text{-}F}$ = 251.6 Hz), 145.3, 145.2 (d, $J_{C\text{-}F}$ = 11.7 Hz), 135.4, 131.2 (d, $J_{C\text{-}F}$ = 11.6 Hz), 130.2, 130.1, 130.0, 129.9, 129.8, 128.2, 127.9, 127.7, 127.5, 127.4, 115.1, 110.9 (d, $J_{C\text{-}F}$ = 23.1 Hz), 102.0 (d, $J_{C\text{-}F}$ = 27.5 Hz), 84.9, 75.1, 53.7, 46.3, 31.0, 29.7, 21.7, 9.1, 8.8; HRMS (ESI) *m/z*: 407.1806 (Calcd for $C_{21}H_{28}FN_2O_3S$ $[M]^+$: 407.1805).

trans-7-fluoro-2-Hydroxy-1-tosylindoline-3-ammonium bromide (1h)



1h

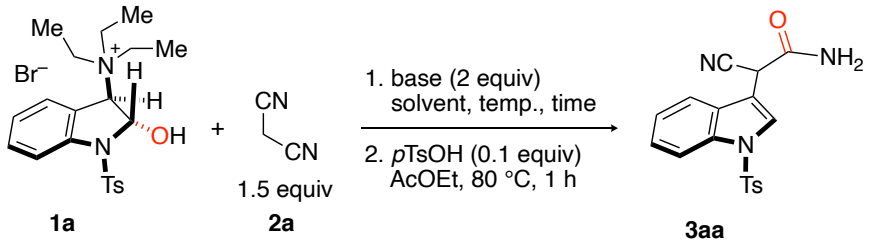
To a solution of 5-fluoro-1-tosylindole (578.7 mg, 2 mmol) and H_2O (0.36 mL, 20 mmol) in acetone (10 mL) was added NBS (355.9 mg, 2.0 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material as indicated by TLC. Et_3N (0.28 mL, 2.0 mmol) was added to the mixture and stirred further 1 h. Then, Et_2O (5 mL) was added to the mixture at room temperature and stirred further 1h. The resulting precipitate was

separated by filtration, washed with acetone/Et_2O (1/1), and dried *in vacuo* to give **1h** (828.6 mg, 85% yield).

828.6 mg, 85% yield. colorless solid; mp: 159.7-161.7 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 8.22 (br s, 1H), 7.92 (d, J = 7.8 Hz, 2H), 7.47 (d, J = 7.8 Hz, 1H), 7.44 (d, J = 7.8 Hz, 2H), 7.33-7.38 (m, 1H), 7.19-7.24 (m, 1H), 6.53 (s, 1H), 4.90 (s, 1H), 3.50–3.61 (m, 6H), 2.38 (s, 3H), 1.17 (t, J = 7.2 Hz, 9H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 150.2 (d, $J_{C\text{-}F}$ = 250.2 Hz), 144.8, 137.7, 130.5 (d, $J_{C\text{-}F}$ = 11.6 Hz), 130.3, 127.6, 126.8, 126.3 (d, $J_{C\text{-}F}$ = 5.7 Hz), 125.5, 120.5 (d, $J_{C\text{-}F}$ = 18.9 Hz), 86.0, 74.5, 53.7, 46.1, 21.6, 9.1, 9.0; HRMS (ESI) *m/z*: 407.1788 (Calcd for $C_{21}H_{28}FN_2O_3S$ $[M]^+$: 407.1805).

■Optimization of Reaction Conditions

Table S1 Optimization of telescoping reaction conditions [a]



run	base	solvent	temp. (° C)	time (h)	yield (%)[b]
1	Et_3N	AcOEt	80	2	71
2	Et_3N	THF	80	2	73
3	Et_3N	1,4-dioxane	80	2	52
4	Et_3N	DME	80	2	58
5	Et_3N	CPME	80	2	47
6	Et_3N	toluene	80	2	61
7	Et_3N	benzene	80	2	68
8	**Et_3N**	**ClC_6H_5**	**80**	**2**	**88**
9	Et_3N	DCM	50	2	0
10	Et_3N	DCE	80	2	81
11	Et_3N	$CHCl_3$	80	2	72
12	Et_3N	DMSO	80	2	70
13	Et_3N	DMF	80	2	83
14	iPr_2NEt	ClC_6H_5	80	2	68
15	pyridine	ClC_6H_5	80	2	51
16	DMAP	ClC_6H_5	80	2	7
17	NaOH	ClC_6H_5	80	2	58
18	KOH	ClC_6H_5	80	2	50
19	Cs_2CO_3	ClC_6H_5	80	2	14
20[c]	------	**ClC_6H_5**	**80**	**19**	**92**

[a] **1a** (0.5 mmol), malononitrile **2a** (0.75 mmol), and base (1.0 mmol) in solvent (5 mL). [b] Isolated yields. [c] Without performing 2nd step (*p*TsOH, AcOEt, 80 °C, 1 h).

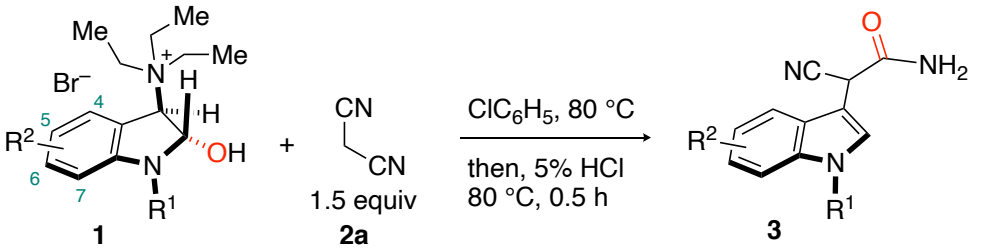
■General procedure A (Table S1)

A mixture of **1a** (234.7 mg, 0.5 mmol), **2a** (49.6 mg, 0.75 mmol) and base (1.0 mmol) in solvent (5 mL) was heated at the indicated temperature (oil-bath) with stirring for 2–16 h. After cooling to room temperature, water was added to the mixture and the whole was extracted with AcOEt (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo* to afford crude material which was dissolved in AcOEt (5 mL). To this solution was added *p*TsOH (0.05 mmol) and the mixture was heated at 80 °C with stirring for 1 h. After addition of water at room temperature, the whole was extracted with AcOEt (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo* The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5–1:1) to give **3aa**.

■General procedure B (Table S1)

A mixture of **1a** (234.7 mg, 0.5 mmol) and **2a** (49.6 mg, 0.75 mmol) in ClC_6H_5 (5 mL) was heated at 80 °C (oil-bath) with stirring. After 2 h, to this solution was added acid and the mixture was heated at 80 °C with stirring for 0.5–1 h. After addition of water at room temperature, the whole was extracted with AcOEt (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo* The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5–1:1) to give **3aa**.

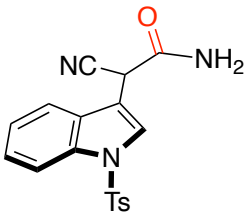
■General procedure C (Scheme 2)



1a: R^1 = Ts, R^2 = H
1b: R^1 = Ts, R^2 = 5-MeO
1c: R^1 = Ts, R^2 = 5-Cl
1d: R^1 = Ts, R^2 = 5-Br
1e: R^1 = Ts, R^2 = 5-F
1f: R^1 = Ts, R^2 = 4-F
1g: R^1 = Ts, R^2 = 6-F
1h: R^1 = Ts, R^2 = 7-F
1i: R^1 = Bs, R^2 = H

A mixture of **1** (1 mmol) and **2a** (99.1 mg, 1.5 mmol) in ClC_6H_5 (10 mL) was heated at 80 °C (oil-bath) with stirring. After 2 h, to this solution was added 5% HCl (5 mL) and the mixture was heated at 80 °C with stirring for 0.5 h. After addition of water at room temperature, the whole was extracted with AcOEt (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5–1:1) to give **3aa-3ia**.

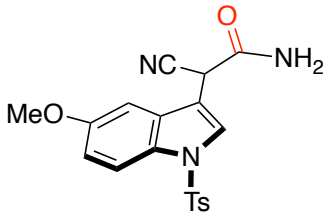
2-Cyano-2-(1-tosyl-1*H*-indol-3-yl)acetamide (3aa)



3aa

General procedure C: 349.9 mg, 99% yield. colorless solid; mp: 173.3-176.0 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.89 (d, J = 7.8 Hz, 1H), 7.88 (d, J = 8.4 Hz, 2H), 7.82 (d, J = 2.4 Hz, 1H), 7.77 (br s, 1H), 7.64 (d, J = 7.8 Hz, 1H), 7.57 (br s, 1H), 7.35–7.38 (m, 2H), 7.36 (t, J = 6.3 Hz, 1H), 7.29 (t, J = 7.8 Hz, 1H), 5.39 (s, 1H), 2.28, 2.29 (2 s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 165.4, 146.5, 134.7, 134.3, 130.9, 128.4, 127.5, 126.5, 126.0, 124.2, 120.6, 117.5, 113.8, 113.7, 36.4, 21.6; HRMS (ESI) *m/z*: 376.0723 (Calcd for $C_{18}H_{15}N_3NaO_3S$ $[M+Na]^+$: 376.0732).

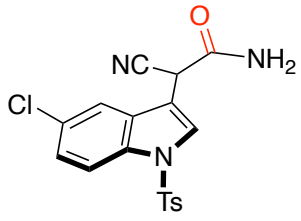
2-Cyano-2-(5-methoxy-1-tosyl-1*H*-indol-3-yl)acetamide (3ba)



3ba

General procedure C: 254.6 mg, 66% yield. colorless solid; mp: 163.7-164.2 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.83 (d, J = 8.4 Hz, 2H), 7.79 (br s, 1H), 7.79 (d, J = 9.0 Hz, 1H), 7.75 (s, 1H), 7.57 (br s, 1H), 7.36 (d, J = 8.4 Hz, 2H), 7.11 (d, J = 2.4 Hz, 1H), 6.98 (dd, J = 2.4, 9.0 Hz, 1H), 5.33 (s, 1H), 3.71 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 165.4, 156.6, 146.3, 134.3, 130.9, 129.5, 129.3, 127.4, 127.2, 117.5, 114.8, 114.5, 113.9, 103.4, 56.1, 36.3, 21.6; HRMS (ESI) *m/z*: 406.0822 (Calcd for $C_{19}H_{17}N_3NaO_4S$ $[M+Na]^+$: 406.0837).

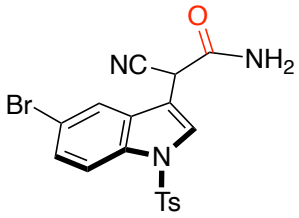
2-(5-Chloro-1-tosyl-1*H*-indol-3-yl)-2-cyanoacetamide (3ca)



3ca

General procedure C: 309.0 mg, 80% yield. colorless solid; mp: 198.8-202.3 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.93 (d, J = 8.4 Hz, 1H), 7.89–7.90 (m, 3H), 7.84 (br s, 1H), 7.67 (d, J = 1.8 Hz, 1H), 7.61 (br s, 1H), 7.41 (dd, J = 1.8, 9.0 Hz, 1H), 7.38 (d, J = 9.0 Hz, 2H), 5.38 (d, J = 1.2 Hz, 1H), 2.30 (s, 3H);^{13}C NMR (151 MHz, DMSO-d_6) δ: 165.3, 146.8, 134.1, 133.2, 131.0, 129.7, 128.9, 128.1, 127.6, 126.0, 120.0, 117.4, 115.6, 113.2, 36.2, 21.6; HRMS (ESI) *m/z*: 410.0334, 412.0311 (Calcd for $C_{18}H_{14}ClN_3NaO_3S$ $[M+Na]^+$: 410.0342, 412.0311).

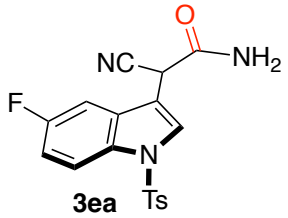
2-(5-Bromo-1-tosyl-1*H*-indol-3-yl)-2-cyanoacetamide (3da)



3da

General procedure C: 317.4 mg, 73% yield. colorless solid; mp: 197.8-200.8 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.82-7.90 (m, 6H), 7.62 (br s, 1H), 7.52 (d, J = 9.0 Hz, 1H), 7.37 (m, 2H), 5.39–5.40 (m, 1H), 2.28, 2.29 (2 s, 3H);^{13}C NMR (151 MHz, DMSO-d_6) δ: 165.3, 146.7, 134.0, 133.5, 131.0, 130.2, 128.6, 128.0, 127.5, 123.0, 117.4, 116.9, 115.9, 113.1, 36.2, 21.6; HRMS (ESI) *m/z*: 453.9840, 455.9819 (Calcd for $C_{18}H_{14}BrN_3NaO_3S$ $[M+Na]^+$: 453.9837, 455.9816).

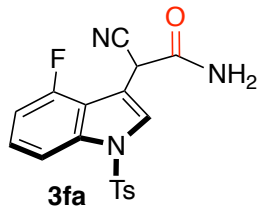
2-Cyano-2-(5-fluoro-1-tosyl-1*H*-indol-3-yl)acetamide (3ea)



3ea

General procedure C: 344.7 mg, 93% yield. colorless solid; mp: 185.8-186.8 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.94 (dd, J = 3.6, 8.4 Hz, 1H), 7.80 (s, 1H), 7.78 (d, J = 7.8 Hz, 2H), 7.29 (dd, J = 2.4, 9.0 Hz, 1H), 7.28 (d, J = 7.8 Hz, 2H), 7.12 (td, J = 2.4, 9.0 Hz, 1H), 5.97 (br s, 1H), 5.68 (br s, 1H), 4.78 (s, 1H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 164.0, 159.9 (d, $J_{C\text{-}F}$ = 242.8 Hz), 146.1, 134.5, 131.6, 130.4, 128.6 (d, $J_{C\text{-}F}$ = 10.1 Hz), 127.2, 127.1, 115.5, 115.2 (d, $J_{C\text{-}F}$ = 8.7 Hz), 114.3 (d, $J_{C\text{-}F}$ = 24.6 Hz), 111.5 (d, $J_{C\text{-}F}$ = 4.4 Hz), 105.6 (d, $J_{C\text{-}F}$ = 24.6 Hz), 36.5, 21.8; HRMS (ESI) *m/z*: 394.0638 (Calcd for $C_{18}H_{14}FN_3NaO_3S$ $[M+Na]^+$: 394.0638).

2-Cyano-2-(4-fluoro-1-tosyl-1*H*-indol-3-yl)acetamide (3fa)

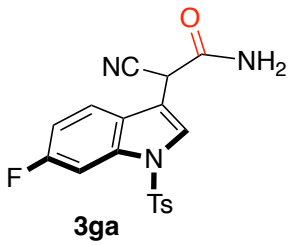


3fa

General procedure C: 305.7 mg, 82% yield. colorless solid; mp: 165.1-166.4 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.93 (d, J = 8.4 Hz, 2H), 7.81 (s, 1H), 7.74 (d, J = 8.4 Hz, 1H), 7.66 (br s, 1H), 7.61 (br s, 1H), 7.40 (d, J = 7.8 Hz, 2H), 7.34-7.38 (m, 1H), 7.08 (dd, J = 7.8, 9.6 Hz, 1H), 5.47, 5.50 (2s, 1H), 2.31 (s, 3H) (containing rotamers); ^{13}C NMR (151 MHz, $CDCl_3$) δ:165.3, 165.1, 165.0, 155.8 (d, $J_{C\text{-}F}$ = 248.7 Hz), 151.8 (d, $J_{C\text{-}F}$ = 248.7 Hz), 147.0, 146.8, 136.8 (d, $J_{C\text{-}F}$ = 8.8 Hz), 135.9 (d, $J_{C\text{-}F}$ = 8.6 Hz), 134.1, 133.9, 131.1, 131.0, 130.0, 128.5, 127.7, 127.6, 127.2, 118.4 (d, $J_{C\text{-}F}$ = 20.2 Hz), 117.7, 117.6, 117.2 (d, $J_{C\text{-}F}$ = 21.6 Hz), 115.9, 115.2, 114.8, 111.6 (d, $J_{C\text{-}F}$ = 2.9 Hz), 111.5 (d, $J_{C\text{-}}$

$_F$ = 2.9 Hz), 111.3, 110.2,109.8 (d, $J_{C\text{-}F}$ = 18.9 Hz), 102.4 (d, $J_{C\text{-}F}$ = 18.9 Hz), 36.2, 36.1, 22.7, 21.6 (containing rotamers); HRMS (ESI) *m/z*: 394.0635 (Calcd for $C_{18}H_{14}FN_3NaO_3S$ $[M+Na]^+$: 394.0638).

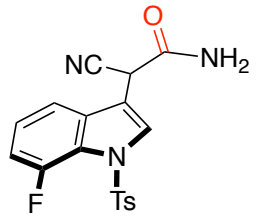
2-Cyano-2-(6-fluoro-1-tosyl-1*H*-indol-3-yl)acetamide (3ga)



3ga

General procedure C: 318.3 mg, 86% yield. colorless solid; mp: 181.8-187.8 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.80 (d, *J* = 8.4 Hz, 2H), 7.75 (s, 1H), 7.22 (dd, *J* = 3.0, 9.0 Hz, 1H), 7.57 (dd, *J* = 5.4, 9.6 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.06 (td, *J* = 3.0, 9.0 Hz, 1H), 5.90 (br s, 1H), 5.53 (br s, 1H), 4.80 (s, 1H), 2.38 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 164.2, 161.6 (d, $J_{C\text{-}F}$ = 245.8 Hz), 146.2, 135.5 (d, $J_{C\text{-}F}$ = 19.6 Hz), 134.5, 130.5, 127.1, 125.8, 123.9, 120.9 (d, $J_{C\text{-}F}$ = 10.1 Hz), 115.6, 112.8 (d, $J_{C\text{-}F}$ = 24.6 Hz), 111.7, 101.3 (d, $J_{C\text{-}F}$ = 27.5 Hz), 36.7, 21.8; HRMS (ESI) *m/z*: 394.0636 (Calcd for $C_{18}H_{14}FN_3NaO_3S$ $[M+Na]^+$: 394.0638).

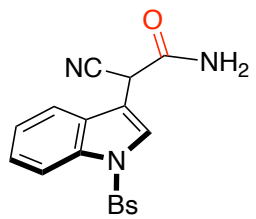
2-Cyano-2-(7-fluoro-1-tosyl-1*H*-indol-3-yl)acetamide (3ha)



3ha

General procedure C: 333.5 mg, 90% yield. colorless solid; mp: 88.2-91.6 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.97 (s, 1H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.77 (br s, 1H), 7.61 (br s, 1H), 7.46 (dd, *J* = 1.2, 7.8 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.28 (td, *J* = 4.2, 7.8 Hz, 1H), 7.16 (dd, *J* = 7.8, 12.6 Hz, 1H), 5.49 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 165.4, 149.3 (d, $J_{C\text{-}F}$ = 250.1 Hz), 146.5, 134.8, 132.6, 130.9, 130.8 (d, $J_{C\text{-}F}$ = 7.3 Hz), 129.3, 127.9, 125.5 (d, $J_{C\text{-}F}$ = 7.3 Hz), 121.8 (d, $J_{C\text{-}F}$ = 11.5 Hz), 117.4, 116.7, 112.5 (d, $J_{C\text{-}F}$ = 24.5 Hz), 112.3, 36.3, 21.6; HRMS (ESI) *m/z*: 394.0642 (Calcd for $C_{18}H_{14}FN_3NaO_3S$ $[M+Na]^+$: 394.0638).

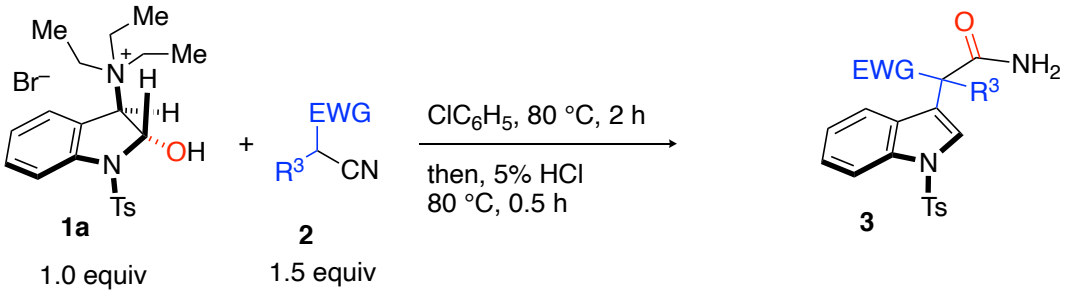
2-(1-Benzenesulfonyl-1*H*-indol-3-yl)-2-cyanoacetamide (3ia)



3ia

General procedure C: 277.9 mg, 82% yield. colorless solid; mp: 191.8-194.8 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 8.00 (dd, J = 1.2, 9.0 Hz, 2H), 7.91 (d, J = 8.4 Hz, 1H), 7.84 (s, 1H), 7.77 (br s, 1H), 7.69 (t, J = 7.8 Hz, 1H), 7.64 (d, J = 7.8 Hz, 1H), 7.57-7.60 (m, 3H), 7.38 (td, J = 1.2, 7.8 Hz, 1H), 7.30 (td, J = 1.2, 7.5 Hz, 1H), 5.39 (s, 1H);^{1} ^{3}C NMR (151 MHz, DMSO-d_6) δ: 165.4, 137.3, 135.5, 134.7, 130.6, 128.4, 127.5, 126.6, 126.1, 124.3, 120.7, 117.5, 114.0, 113.9, 36.3; HRMS (ESI) *m/z*: 362.0575 (Calcd for $C_{17}H_{13}N_3NaO_3S$ $[M+Na]^+$: 362.0580).

■General procedure D1 (Scheme 3)



EWG / CN

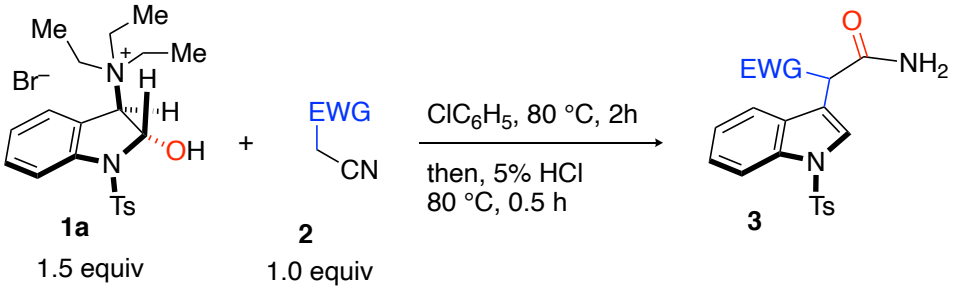
2a: EWG = CN
2b: EWG = CO_2Me
2c: EWG = CO_2Et
2d: EWG = CO_2iPr
2e: EWG = $CO_2CH_2CH_2OEt$
2f: EWG = Bs
2g: EWG = Ts
2h: EWG = Ms
2i: EWG = Bz
2j: EWG = CO-(4-FC_6H_4)
2k: EWG = CO-(3-ClC_6H_4)
2l: EWG = CO-(2-ClC_6H_4)
2m: EWG = CO-(2-thienyl)
2n: EWG = pivaloyl

EWG / R^3 / CN

2o: R^3 = Me, EWG = CN
2p: R^3 = Ph, EWG = CO_2Et

A mixture of **1a** (469.4 mg, 1 mmol) and **2** (1.5 mmol) in ClC_6H_5 (10 mL) was heated at 80 °C (oil-bath) with stirring. After 2 h, to this solution was added 5% HCl (5 mL) and the mixture was heated at 80 °C with stirring for 0.5 h. After addition of water at room temperature, the whole was extracted with AcOEt (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5–1:1-3:1) to give **3ab**, **3ac**, **3ad**, **3ae**, **3af**, **3ag**, **3ah**, **3an**, **3ao**, and **3ap**.

■General procedure D2 (Scheme 3)

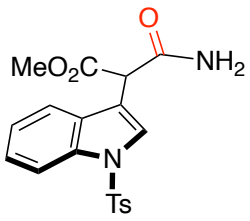


2j: EWG = CO-(4-FC_6H_4)
2k: EWG = CO-(3-ClC_6H_4)
2l: EWG = CO-(2-ClC_6H_4)
2m: EWG = CO-(2-thienyl)

A mixture of **1a** (704.1 mg, 1.5 mmol) and **2** (1.0 mmol) in ClC_6H_5 (10 mL) was heated at 80 °C (oil-bath) with

stirring. After 2 h, to this solution was added 5% HCl (5 mL) and the mixture was heated at 80 °C with stirring for 0.5 h. After addition of water at room temperature, the whole was extracted with AcOEt (3 x 20 mL), washed with brine (20 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5–1:1-3:1) to give **3aj**, **3ak**, **3al**, and **3am**.

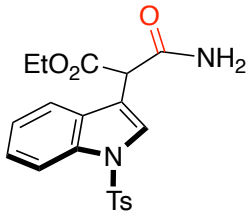
Methyl 3-amino-3-oxo-2-(1-tosyl-1*H*-indol-3-yl)propanoate (3ab)



3ab

General procedure D1: 80.0 mg, 21% yield. colorless solid; mp: 138.7-141.7 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.74 (s, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.33 (td, *J* = 1.2, 9.0 Hz, 1H), 7.26 (td, *J* = 0.6, 6.0 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 6.53 (br s, 1H), 6.17 (br s, 1H), 4.74 (s, 1H), 3.78 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 169.8, 169.4, 145.5, 135.0, 130.2, 129.1, 127.1, 125.5, 125.2, 123.8, 119.9, 114.8, 113.8, 53.3, 50.1, 21.7; HRMS (ESI) *m/z*: 409.0829 (Calcd for $C_{19}H_{18}N_2NaO_5S$ $[M+Na]^+$: 409.0834).

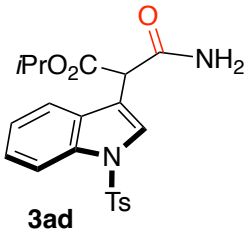
Ethyl 3-amino-3-oxo-2-(1-tosyl-1*H*-indol-3-yl)propanoate (3ac)



3ac

General procedure D1: 81.3 mg, 20% yield. colorless solid; mp: 138.7-141.7 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.74 (s, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.33 (td, *J* = 1.2, 7.8 Hz, 1H), 7.25 (t, *J* = 7.2 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 2H), 6.55 (br s, 1H), 6.01 (br s, 1H), 4.71 (s, 1H), 4.19-4.27 (m, 2H), 2.33 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ:169.4, 169.0, 145.4, 135.0, 130.1, 129.2, 127.0, 125.5, 125.0, 123.7, 120.0, 115.3, 113.7, 62.4, 50.4, 21.7, 14.1; HRMS (ESI) *m/z*: 423.0989 (Calcd for $C_{20}H_{20}N_2NaO_5S$ $[M+Na]^+$: 423.0991).

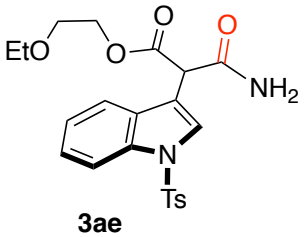
Isopropyl 3-amino-3-oxo-2-(1-tosyl-1*H*-indol-3-yl)propanoate (3ad)



3ad

General procedure D1: 49.7 mg, 12% yield. colorless solid; mp: 152.2-156.2 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.96 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.71 (s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.33 (td, *J* = 1.2, 7.8 Hz, 1H), 7.25 (td, *J* = 1.2, 8.4 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 6.55 (br s, 1H), 5.62 (br s, 1H), 5.09 (sept, *J* = 6.0 Hz, 1H), 4.66 (s, 1H), 2.33 (s, 3H), 1.27 (d, *J* = 6.0 Hz, 3H), 1.19 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 169.1, 168.6, 145.4, 135.1, 130.1, 129.3, 127.0, 125.5, 123.7, 120.0, 115.7, 113.8, 70.2, 50.7, 21.7, 21.6; HRMS (ESI) *m/z*: 437.1136 (Calcd for $C_{21}H_{22}N_2NaO_5S$ $[M+Na]^+$: 437.1147).

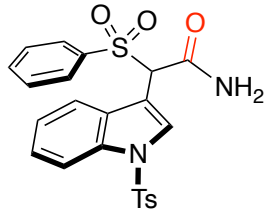
2-Ethoxyethyl 3-amino-3-oxo-2-(1-tosyl-1*H*-indol-3-yl)propanoate (3ae)



3ae

General procedure D1: 101.8 mg, 23% yield. colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.76 (s, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.26 (t, *J* = 8.4 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 2H), 6.52 (br s, 1H), 5.42 (br s, 1H), 4.77 (s, 1H), 4.35 (t, *J* = 3.6 Hz, 2H), 3.63 (q, *J* = 4.8 Hz, 2H), 3.47 (q, *J* = 6.6 Hz, 2H), 2.34 (s, 3H), 1.15 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 169.2, 168.6, 145.3, 135.1, 135.0, 130.1, 129.3, 127.0, 125.4, 125.2, 123.7, 120.0, 115.2, 113.7, 68.0, 66.7, 65.2, 50.5, 21.7, 15.1; HRMS (ESI) *m/z*: 467.1249 (Calcd for $C_{22}H_{24}N_2NaO_6S$ $[M+Na]^+$: 467.1253).

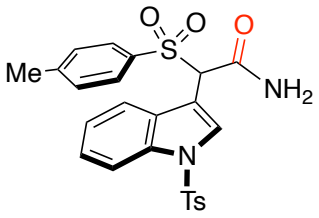
2-(Phenylsulfonyl)-2-(1-tosyl-1*H*-indol-3-yl)acetamide (3af)



3af

General procedure D1: 168.7 mg, 36% yield. colorless solid; mp: 238.6-239.9 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.84 (d, *J* = 8.4 Hz, 1H), 7.79 (br s, 1H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.63 (s, 1H), 7.61 (t, *J* = 8.1 Hz, 2H), 7.41-7.45 (m, 5H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.30 (t, *J* = 7.2 Hz, 1H), 7.19 (t, *J* = 7.2 Hz, 1H), 5.77 (s, 1H), 2.32 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 165.0, 146.5, 137.0, 134.8, 134.3, 133.8, 131.0, 129.8, 129.5, 129.3, 127.7, 127.2, 125.8, 124.0, 120.3, 113.6, 111.4, 66.2, 21.6; HRMS (ESI) *m/z*: 491.0687 (Calcd for $C_{23}H_{20}N_2NaO_5S_2$ $[M+Na]^+$: 491.0711).

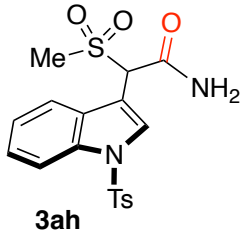
2-Tosyl-2-(1-tosyl-1*H*-indol-3-yl)acetamide (3ag)



3ag

General procedure D1: 241.8 mg, 50% yield. colorless solid; mp: 230.0-234.5 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.92 (d, *J* = 9.0 Hz, 1H), 7.75 (d, *J* = 9.0 Hz, 2H), 7.75 (s, 1H), 7.40 (d, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.27 (td, *J* = 1.2, 7.8 Hz, 1H), 7.24 (d, *J* = 9.0 Hz, 2H), 7.14 (t, *J* = 8.4 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 6.84 (br s, 1H), 5.71 (br s, 1H), 5.21 (s, 1H), 2.35 (s, 3H), 2.30 (s, 3H);$^{1\ 3}$C NMR (151 MHz, $CDCl_3$) δ: 164.3, 145.9, 145.5, 135.0, 134.8, 134.3, 132.6, 130.1, 129.6, 129.5, 129.0, 127.8, 127.1, 125.2, 123.6, 119.4, 113.6, 110.1, 68.1, 21.7, 21.1; HRMS (ESI) *m/z*: 505.0864 (Calcd for $C_{24}H_{22}N_2NaO_5S_2$ $[M+Na]^+$: 505.0868).

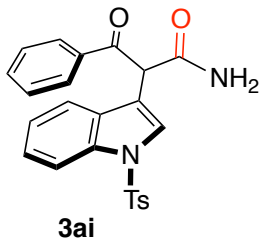
2-(Methylsulfonyl)-2-(1-tosyl-1*H*-indol-3-yl)acetamide (3ah)



3ah

General procedure D1: 48.8 mg, 12% yield. colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.10 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.36 (td, *J* = 1.8, 7.5 Hz, 1H), 7.30 (s, 1H), 7.26 (t, *J* = 7.8 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.86 (br s, 1H), 6.54 (s, 1H), 6.05 (br s, 1H), 3.06 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 163.9, 145.8, 137.3, 134.4, 130.1, 129.0, 127.7, 127.0, 126.3, 124.6, 122.0, 116.2, 115.4, 66.2, 40.5, 21.7; HRMS (ESI) *m/z*: 429.0557 (Calcd for $C_{18}H_{18}N_2NaO_5S_2$ $[M+Na]^+$: 429.0555).

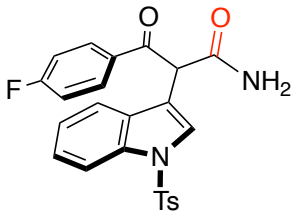
3-Oxo-3-phenyl-2-(1-tosyl-1*H*-indol-3-yl)propenamide (3ai)



3ai

General procedure D1: 320.5 mg, 74% yield. colorless solid; mp: 223.3-227.4 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 8.02 (d, *J* = 7.2 Hz, 2H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.82 (s, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.70 (s, 1H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.51 (d, *J* = 7.8 Hz, 2H), 7.27-7.33 (m, 4H), 7.20 (t, *J* = 7.8 Hz, 1H), 5.95 (s, 1H), 2.33, 2.27 (2s, 3H) (containing keto-enol tautomers); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 194.0, 169.3, 146.1, 136.3, 134.6, 134.5, 134.0, 130.8, 130.7, 130.5, 129.3, 129.0, 128.1, 128.0, 127.2, 127.1, 126.4, 125.3, 123.8, 123.7, 121.6, 117.4, 113.5, 52.6, 21.6 (containing keto-enol tautomers); HRMS (ESI) *m/z*: 455.1041 (Calcd for $C_{24}H_{20}N_2NaO_4S$ $[M+Na]^+$: 455.1041).

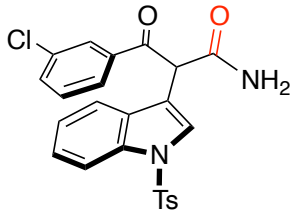
3-(4-Fluorophenyl)-3-oxo-2-(1-tosyl-1*H*-indol-3-yl)propenamide (3aj)



3aj

General procedure D2: 378.4 mg, 84% yield. colorless solid; mp: 200.8-203.8 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.00-8.04 (m, 1.4H), 7.97 (d, *J* = 7.8 Hz, 0.4H), 7.68 (d, *J* = 8.4 Hz, 0.6H), 7.66 (d, *J* = 7.8 Hz, 0.8H), 7.63 (s, 0.4H), 7.55 (d, *J* = 8.4 Hz, 1.2H), 7.47 (d, *J* = 7.2 Hz, 0.6H), 7.38 (t, *J* = 8.4 Hz, 0.4H), 7.36 (t, *J* = 8.4 Hz, 0.6H), 7.29 (t, *J* = 8.4 Hz, 0.4H), 7.28 (t, *J* = 8.4 Hz, 0.6H), 7.22 (s, 0.6H), 7.18 (d, *J* = 8.4 Hz, 1.2H), 7.15 (d, *J* = 8.4 Hz, 0.8H), 7.06-7.11 (m, 2H), 6.52 (t, *J* = 7.8 Hz, 1H), 6.44 (br s, 0.4H), 5.70 (s, 0.4H), 5.52 (br s, 0.4H), 5.30 (br s, 0.6H), 5.29 (br s, 0.6H), 2.39 (s, 1.8H), 2.32 (s, 1.2H) (containing keto-enol tautomers); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 193.8, 174.6, 172.3, 169.0, 166.4 (d, $J_{C\text{-}F}$ = 257.3 Hz), 163.1 (d, $J_{C\text{-}F}$ = 250.2 Hz), 145.4, 145.3, 135.2, 135.1, 135.0, 134.9, 132.1 (d, $J_{C\text{-}F}$ = 2.9 Hz), 131.8 (d, $J_{C\text{-}F}$ = 10.1 Hz), 131.2 (d, $J_{C\text{-}F}$ = 2.9 Hz), 130.7, 130.2 (d, $J_{C\text{-}F}$ = 8.6 Hz), 130.1, 129.2, 126.9 (d, $J_{C\text{-}F}$ = 10.1 Hz), 126.8, 125.8, 125.7, 125.2, 124.2, 124.0, 120.2, 119.8, 116.7, 116.2, 116.2 (d, $J_{C\text{-}F}$ = 21.7 Hz), 114.8 (d, $J_{C\text{-}F}$ = 21.7 Hz), 114.1, 113.9, 93.0, 52.4, 21.7 (containing keto-enol tautomers); HRMS (ESI) *m/z*: 473.0935 (Calcd for $C_{24}H_{19}FN_2NaO_4S$ $[M+Na]^+$: 473.0947).

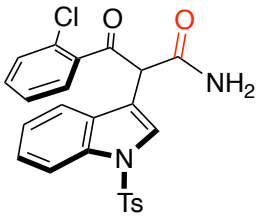
3-(3-Chlorophenyl)-3-oxo-2-(1-tosyl-1*H*-indol-3-yl)propenamide (3ak)



3ak

General procedure D2: 401.6 mg, 86% yield. colorless solid; mp: 192.8-194.8 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.97 (d, *J* = 9.0 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 7.2 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.25-7.27 (m, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.10 (dd, *J* = 2.4, 4.2 Hz, 1H), 6.88 (d, *J* = 8.4 Hz, 1H), 6.77 (t, *J* = 8.4 Hz, 1H), 5.55 (br s, 1H), 5.36 (br s, 1H), 2.37 (s, 3H) (containing keto-enol tautomers); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 194.2, 174.7, 171.6, 169.1, 145.4, 145.3, 137.3, 136.9, 135.4, 135.2, 135.1, 135.0, 134.8, 134.1, 133.9, 130.5, 130.3, 130.2, 130.1, 129.6, 129.1, 129.0, 128.9, 128.2, 127.1, 127.0, 126.9, 126.8, 126.2, 125.8, 125.7, 125.3, 124.1, 124.0, 93.7, 52.5, 21.8, 21.7 (containing keto-enol tautomers); HRMS (ESI) *m/z*: 489.0644, 491.0622 (Calcd for $C_{24}H_{19}ClN_2NaO_4S$ $[M+Na]^+$: 489.0652, 491.0622).

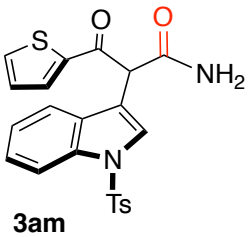
3-(2-Chlorophenyl)-3-oxo-2-(1-tosyl-1*H*-indol-3-yl)propenamide (3al)



3al

General procedure D2: 303.5 mg, 65% yield. colorless solid; mp: 209.2-211.7 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.82 (d, *J* = 8.4 Hz, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.33 (s, 1H), 7.27 (t, *J* = 8.4 Hz, 1H), 7.23 (td, *J* = 1.2, 6.6 Hz, 1H), 7.17 (d, *J* = 8.4 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 2H), 7.08 (td, *J* = 1.8, 7.8 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 6.91 (t, *J* = 7.8 Hz, 1H), 5.42 (br s, 1H), 5.32 (br s, 1H), 2.35 (s, 3H) (containing keto-enol tautomers); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 174.1, 172.0, 144.9, 135.0, 134.6, 132.2, 130.1, 130.0, 129.9, 129.5, 126.9, 126.7, 126.3, 125.3, 123.7, 120.4, 115.3, 113.6, 96.0, 21.7 (containing keto-enol tautomers); HRMS (ESI) *m/z*: 489.0641, 491.0620 (Calcd for $C_{24}H_{19}ClN_2NaO_4S$ $[M+Na]^+$: 489.0652, 491.0622).

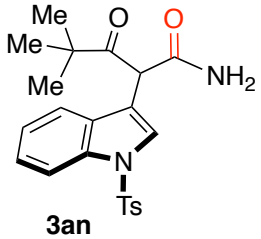
3-Oxo-3-(thiophen-2-yl)-2-(1-tosyl-1*H*-indol-3-yl)propenamide (3am)



3am

General procedure D2: 285.0 mg, 65% yield. colorless solid; mp: 219.8-222.8 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.11 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.59 (s, 1H), 7.40 (t, *J* = 7.2 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.22-7.25 (m, 3H), 7.11 (dd, *J* = 1.2, 3.0 Hz, 1H), 6.97 (dd, *J* = 1.2, 4.8 Hz, 1H), 6.69 (dd, *J* = 3.6, 4.8 Hz, 1H), 5.20 (br s, 1H), 5.16 (br s, 1H), 2.40 (s, 3H) (containing keto-enol tautomers); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 174.8, 165.9, 145.4, 145.3, 136.7, 136.2, 135.7, 135.6, 134.2, 131.0, 130.5, 130.3, 130.1, 129.8, 128.8, 128.7, 128.0, 127.3, 127.0, 126.9, 126.7, 125.8, 125.0, 124.1, 123.9, 123.6, 120.2, 119.9, 119.8, 119.4, 115.9, 114.1, 114.0, 113.9, 90.3, 53.5, 21.8, 21.7 (containing keto-enol tautomers); HRMS (ESI) *m/z*: 461.0606 (Calcd for $C_{22}H_{18}N_2NaO_4S_2$ $[M+Na]^+$: 461.0606).

4,4-Dimethyl-3-oxo-2-(1-tosyl-1*H*-indol-3-yl)pentanamide (3an)

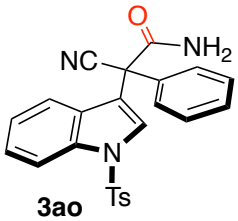


3an

General procedure D1: 115.5 mg, 28% yield. colorless solid; mp: 158.7-161.7 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ:

7.97 (d, J = 8.4 Hz, 1H), 7.72 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.4 Hz, 1H), 7.52 (s, 1H), 7.34 (t, J = 7.8 Hz, 1H), 7.26 (t, J = 7.2 Hz, 1H), 7.20 (d, J = 7.8 Hz, 2H), 6.33 (br s, 1H), 5.75 (br s, 1H), 5.26 (s, 1H), 2.32 (s, 3H), 1.15 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 211.1, 169.5, 145.4, 135.3, 135.0, 130.1, 129.2, 126.9, 125.7, 124.6, 123.9, 119.9, 116.9, 113.9, 51.1, 46.0, 25.9, 21.7; HRMS (ESI) *m/z*: 435.1349 (Calcd for $C_{22}H_{24}N_2NaO_4S$ $[M+Na]^+$: 435.1354).

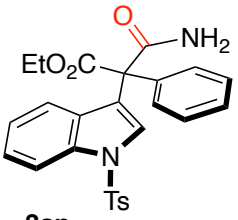
2-Cyano-2-phenyl-2-(1-tosyl-1*H*-indol-3-yl)acetamide (3ao)



3ao

General procedure D1: 347.9 mg, 81% yield. colorless solid; mp: 62.0-68.9 °C;^{1}H NMR (600 MHz, , $CDCl_3$) δ: 7.96 (d, J = 7.8 Hz, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.55 (s, 1H), 7.45-7.48 (m, 2H), 7.36-7.41 (m, 3H), 7.31-7.33 (m, 2H), 7.25 (d, J = 7.8 Hz, 2H), 7.17 (t, J = 6.6 Hz, 1H), 6.45 (br s, 1H), 6.25 (br s, 1H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 167.1, 145.7, 135.5, 134.8, 133.9, 130.3, 129.6, 129.5, 127.6, 127.4, 127.1, 126.8, 125.7, 123.9, 120.7, 118.7, 117.3, 113.9, 53.2, 21.7; HRMS (ESI) *m/z*: 452.1042 (Calcd for $C_{24}H_{19}N_3NaO_3S$ $[M+Na]^+$: 452.1045).

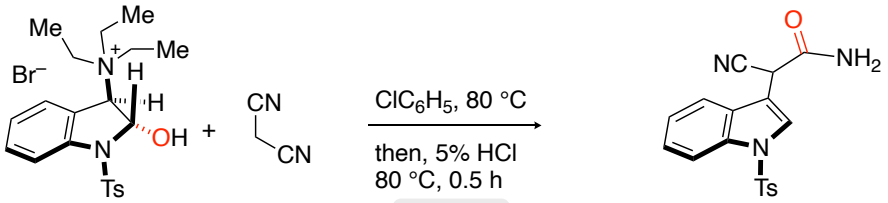
Ethyl 3-amino-3-oxo-2-phenyl-2-(1-tosyl-1*H*-indol-3-yl)propanoate (3ap)



3ap

General procedure D1: 243.1 mg, 51% yield. colorless solid; mp: 129.7-137.7 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.92 (d, J = 8.4 Hz, 1H), 7.72 (d, J = 7.8 Hz, 2H), 7.48 (s, 1H), 7.31-7.36 (m, 5H), 7.22 (d, J = 8.4 Hz, 2H), 7.21-7.24 (m, 1H), 7.07 (t, J = 8.4 Hz, 1H), 7.04 (t, J = 8.4 Hz, 1H), 6.91 (br s, 1H), 5.82 (br s, 1H), 4.19-4.24 (m, 2H), 2.34 (s, 3H), 1.08 (t, J = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 171.3, 170.5, 145.1, 137.2, 135.4, 135.2, 130.0, 129.8, 128.7, 128.5, 128.4, 127.2, 127.0, 124.7, 123.2, 121.7, 121.6, 113.7, 63.9, 62.6, 21.7, 13.8; HRMS (ESI) *m/z*: 499.1304 (Calcd for $C_{26}H_{24}N_2NaO_5S$ $[M+Na]^+$: 499.1304).

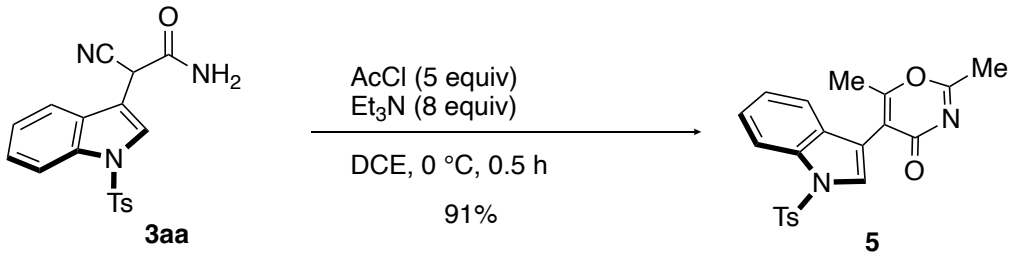
■Procedure for Gram-Scale Synthesis of 3aa (Scheme 4)



1a 4.69 g (10 mmol) **2a** 97% **3aa** 3.41 g

A mixture of **1a** (4.69 g, 10 mmol) and **2a** (991 g, 15 mmol) in ClC_6H_5 (100 mL) was heated at 80 °C with stirring for 2 h. After 2 h, 5% aq. HCl (30 mL) was added to the mixture. Then the mixture was heated at 80 °C for 0.5 h. After cooling to room temperature, the whole was extracted with AcOEt (3 x 200 mL), washed with brine (2 x 100 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5–1:1) to give **3aa** (3.41 g, 97%).

■Synthesis of 5 (Scheme 5)

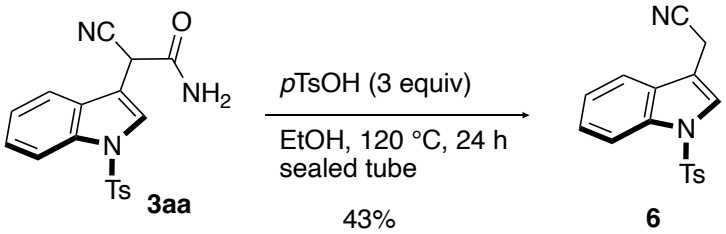


To a solution of **3aa** (70.7 mg, 0.2 mmol) and Et_3N (0.22 mL, 1.6 mmol) in DCE (2 mL) was added AcCl (0.071 mL, 1.0 mmol) at 0 °C under argon atomosphere. The mixture was stirred at 0 °C for 0.5 h. Then, water (5 mL) was added to the mixture and warmed to room temperature. The whole was extracted with AcOEt (2 x 20 mL), washed with brine (2 x 15 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5-1:2) to give **5** (72.0 mg, 91%).

2,6-Dimethyl-5-(1-tosyl-1*H*-indol-3-yl)-4*H*-1,3-oxazin-4-one (5)

5: 72.0 mg, 91% yield. yellow solid; mp: 246.0-248.0 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.97 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.68 (s, 1H), 7.35 (t, *J* = 8.4 Hz, 1H), 7.28 (t, *J* = 6.6 Hz, 1H), 7.24 (d, *J* = 8.4 Hz, 2H), 2.48 (s, 3H), 2.36 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 166.9, 162.3, 145.7, 134.9, 134.5, 130.2, 128.0, 127.0, 125.7, 125.5, 123.9, 120.6, 116.9, 113.6, 111.8, 97.7, 21.7, 21.0, 20.4; HRMS (ESI) *m/z*: 417.0869 (Calcd for $C_{21}H_{18}N_2NaO_4S$ $[M+Na]^+$: 417.0885).

■Synthesis of 6 (Scheme 5)



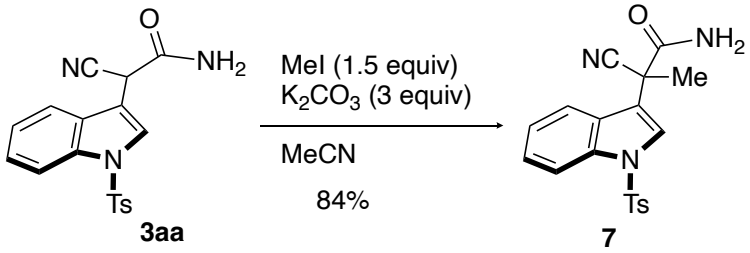
To a solution of **3aa** (35.3 mg, 0.1 mmol) in EtOH (2 mL) was added *p*-TsOH (57.1 mg, 0.3 mmol). The mixture was stirred under reflux conditions (120 °C, oil bath) for 24 h. After cooling to room temperature, water (5 mL) was added to the mixture and the whole was extracted with AcOEt (2 x 20 mL), washed with brine (2 x 15 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:1) to give **6** (13.4 mg, 43%).

2-(1-Tosyl-1*H*-indol-3-yl)acetonitrile (6)[S3]

6: 13.4 mg, 43% yield. colorless solid; mp: 152.7-157.7 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.98 (d, *J* = 9.0 Hz, 1H),

7.77 (d, J = 8.4 Hz, 2H), 7.61 (s, 1H), 7.48 (d, J = 8.4 Hz, 1H), 7.37 (t, J = 7.8 Hz, 1H), 7.29 (t, J = 7.2 Hz, 1H), 7.24 (d, J = 7.8 Hz, 2H), 3.74 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 145.5, 135.2, 135.0, 130.1, 128.8, 127.0, 125.7, 124.5, 123.7, 118.9, 116.8, 114.0, 111.4, 21.7, 14.6.

■Synthesis of 7 (Scheme 5)

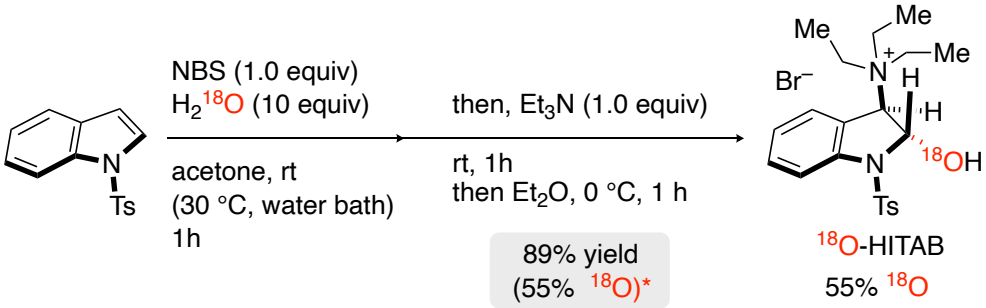


To a solution of **3aa** (35.3 mg, 0.1 mmol) and K_2CO_3 (41.5 mg, 0.3 mmol) in MeCN (1 mL) was added MeI (21.3 mg, 0.15 mmol). The mixture was stirred at room temperature for 2 h. Then, water (5 mL) was added to the mixture and the whole was extracted with AcOEt (2 x 20 mL), washed with brine (2 x 15 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:3-1:1) to give **7** (30.9 mg, 84%).

2-Cyano-2-(1-tosyl-1*H*-indol-3-yl)propenamide (7)

7: 30.9 mg, 84% yield. colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.98 (d, J = 8.4 Hz, 1H), 7.81 (d, J = 8.4 Hz, 2H), 7.74 (s, 1H), 7.67 (d, J = 7.8 Hz, 1H), 7.37 (t, J = 8.4 Hz, 1H), 7.28 (t, J = 6.6 Hz, 1H), 7.27 (d, J = 8.4 Hz, 2H), 5.94 (br s, 1H), 5.73 (br s, 1H), 2.36 (s, 3H), 2.03 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 168.1, 145.8, 135.5, 134.8, 130.3, 127.1, 126.9, 125.9, 124.4, 124.0, 120.3, 119.7, 117.7, 113.9, 42.7, 23.4, 21.8; HRMS (ESI) *m/z*: 390.0888 (Calcd for $C_{19}H_{17}N_3NaO_3S$ $[M+Na]^+$: 390.0888).

■Synthesis of ^{18}O-3aa

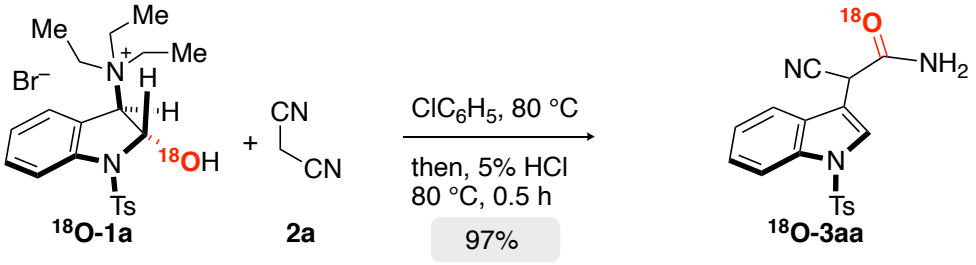


To a solution of 1-tosylindole (1.343 g, 4.95 mmol) and $H_2{}^{18}O$ (1.0 g, 49.5 mmol) in acetone (15 mL) was added NBS (925 mg, 5.198 mmol) under argon atmosphere. The mixture was stirred at 30 °C until the complete disappearance of starting material as indicated by TLC (1 h). Et_3N (0.726 mL, 5.198 mmol) was added to the mixture and stirred under argon atmosphere. After 1h, Et_2O (10 mL) was added to the mixture at 0 °C and stirred further 1h. The resulting precipitate was separated by filtration, washed with acetone/Et_2O (1/1), and dried *in vacuo* to give **^{18}O-1a** (2.07 g, 89% yield).

^{18}O-1a: 2.07 g, 89% yield. colorless solid; mp: 130.6-131.6 °C;^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.89 (d, J = 6.6

Hz, 1H), 8.02 (d, J = 9.0 Hz, 2H), 7.89 (d, J = 7.2 Hz, 1H), 7.54 (t, J = 7.2 Hz, 1H), 7.48 (t, J = 7.2 Hz, 1H), 7.39 (d, J = 8.4 Hz, 2H), 7.13 (t, J = 7.8 Hz, 1H), 6.35 (d, J = 6.6 Hz, 1H), 4.81 (s, 1H), 3.31–3.45 (m, 6H), 2.33 (s, 3H), 1.00 (t, J = 7.8 Hz, 9H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 145.4, 142.8, 136.1, 133.0, 130.5, 130.4, 128.2, 124.0, 120.4, 113.8, 84.7 (**^{16}O, ^{18}O**), 75.4, 53.3, 21.5, 8.8; HRMS (ESI) *m/z*: 389.1889 (**^{16}O**), 391.1930 (**^{18}O**) (Calcd for $C_{21}H_{29}N_2O_3S$ $[M]^+$: 389.1889, $C_{21}H_{29}N_2O_2{}^{18}OS$ $[M]^+$: 391.1941).

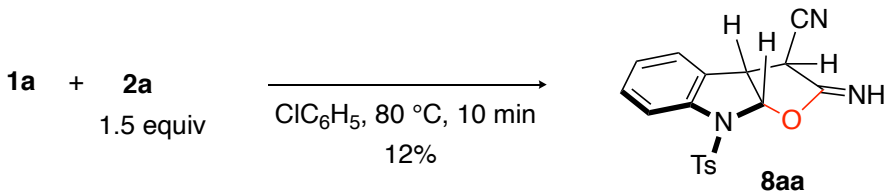
■^{18}O-Incorporation experiment (Scheme 6a)



A mixture of ^{18}O-**1a** (235 mg, 0.5 mmol) and **2a** (49.6 mg, 0.75 mmol) in ClC_6H_5 (5 mL) was heated at 80 °C with stirring for 2 h. After 2 h, 5% aq. HCl (2 mL) was added to the mixture. Then the mixture was heated at 80 °C for 0.5 h. After cooling to room temperature, the whole was extracted with AcOEt (2 x 50 mL), washed with brine (2 x 15 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5–1:1) to give **^{18}O-3aa** (172.4 mg, 97%).

^{18}O-3aa: 172.4 mg, 97% yield. colorless solid; mp: 170.0-173.2 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 7.89 (d, J = 6.6 Hz, 1H), 7.88 (d, J = 9.0 Hz, 2H), 7.81 (s, 1H), 7.77 (br s, 1H), 7.63 (d, J = 7.2 Hz, 1H), 7.57 (br s, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.35–7.38 (m, 1H), 7.29 (t, J = 8.4 Hz, 1H), 5.38 (s, 1H), 2.29 (2 s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 165.29 (**^{16}O**), 165.26 (**^{18}O**), 146.3, 134.9, 134.6, 130.9, 128.5, 127.4, 126.4, 125.9, 124.1, 120.6, 117.4, 114.0, 113.9, 36.2, 21.5; HRMS (ESI) *m/z*: 376.0721 (**^{16}O**), 378.0759 (**^{18}O**) (Calcd for $C_{18}H_{15}N_3NaO_3S$ $[M+Na]^+$: 376.0732, $C_{18}H_{15}N_3NaO_2{}^{18}OS$ $[M+Na]^+$: 378.0774).

■Isolation of the intermediate 8aa (Scheme 6b)

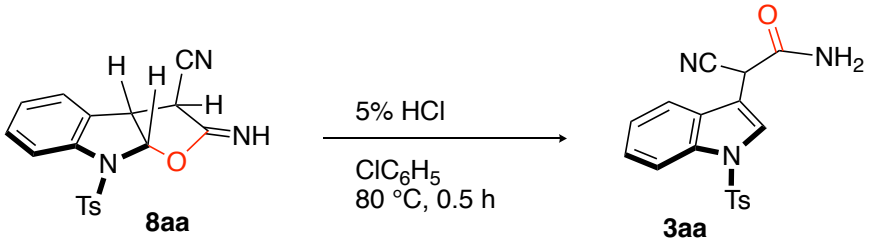


A mixture of **1a** (1.408 g, 3 mmol) and **2a** (297.3 mg, 4.5 mmol) in ClC_6H_5 (30 mL) was heated at 80 °C (oil-bath) with stirring for 10 min. After cooling to room temperature, water was added to the mixture and the whole was extracted with AcOEt (3 x 50 mL), washed with brine (30 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by recrystallization ($CHCl_3$/hexane) to give **8aa** (125.1 mg, 12% yield).

***Rel*-(3*S*,3a*S*,8a*S*)-2-imino-8-tosyl-3,3a,8,8a-tetrahydro-2*H*-furo[2,3-*b*]indole-3-carbonitrile (8aa)**

125.1 mg, 12% yield. colorless solid; mp: 134.2-139.7 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.75 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.23–7.27 (m, 3H), 7.07 (t, *J* = 7.2 Hz, 1H), 6.63 (d, *J* = 7.8 Hz, 1H), 4.67 (br s, 1H), 4.66 (br s, 1H), 4.62 (d, *J* = 7.8 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 167.2, 145.4, 139.0, 134.8, 133.4, 130.6, 129.0, 128.1, 124.9, 124.8, 119.2, 113.9, 96.5, 52.2, 47.6, 21.5; HRMS (ESI) *m/z*: 376.0732 (Calcd for $C_{18}H_{15}N_3NaO_3S$ $[M+Na]^+$: 376.0732).

■The reaction of 8aa (Scheme 6b)

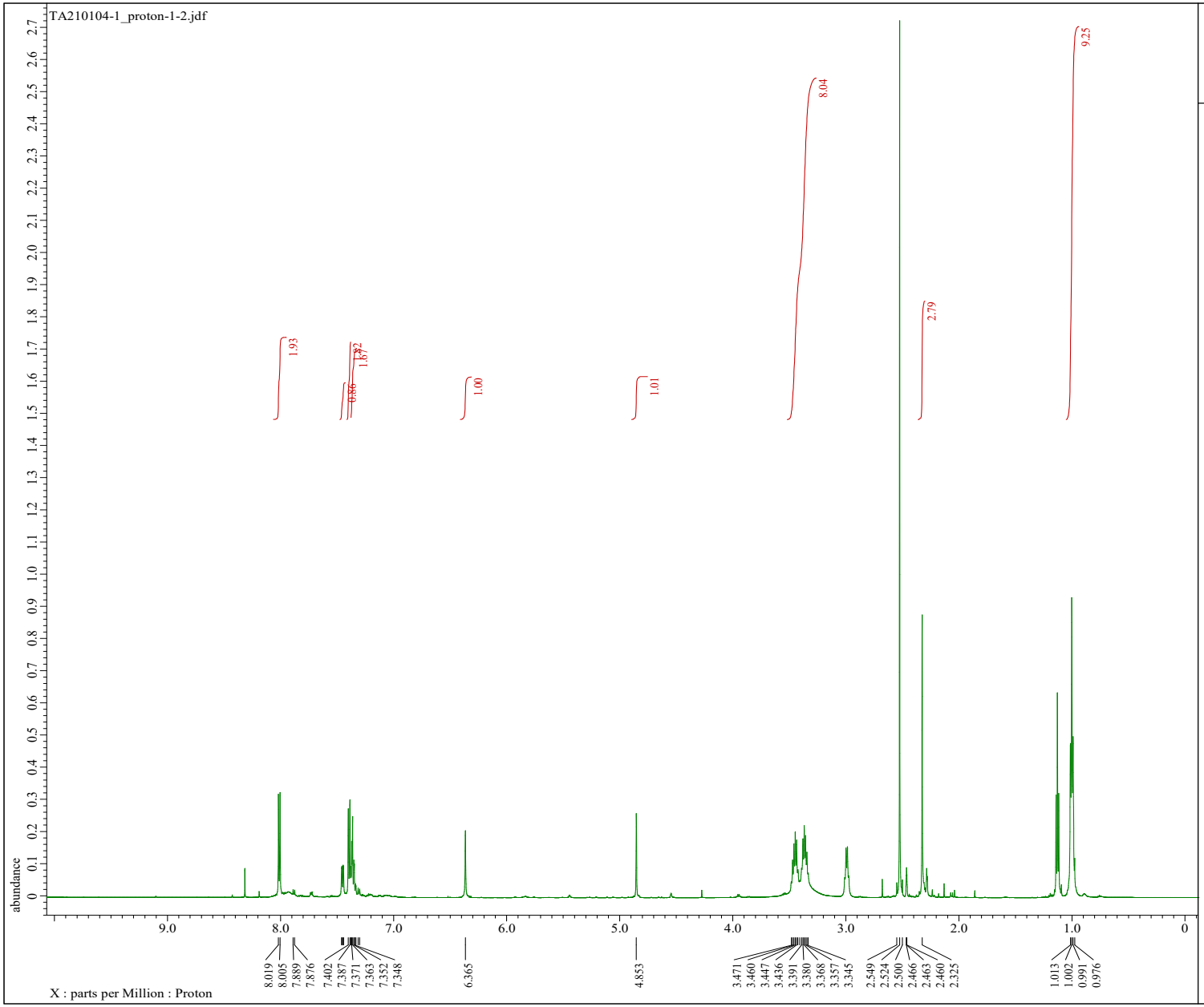


To a solution of **8aa** (106.0 mg, 0.3 mmol) in ClC_6H_5 (3 mL) was added 5% HCl (3 mL) and the mixture was heated at 80 °C with stirring for 0.5 h. After addition of water at room temperature, the whole was extracted with AcOEt (3 x 15 mL), washed with brine (10 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt:hexane = 1:5–1:1-3:1) to give **3aa** (89.2 mg, 84% yield).

(S1) Abe, T.; Suzuki, T.; Anada, M.; Matsunaga, S.; Yamada, K.; *Org. Lett.*, **2017**, *19*, 4275–4278.

(S2) Hirao, S.; Yamashiro, T.; Abe, T. *Chem. Commun*. **2020**, *56,* 10183–10186.

(S3) Chen, X.; Qiu, G.; Liu, R.; Chen, D.; Chen, Z. *Org. Chem. Front*. **2020**, *7,* 890–895.



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Revision_Time         =  4-JAN-2021 20:22:33

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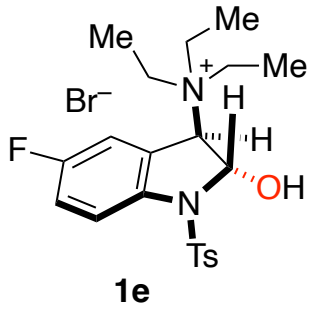

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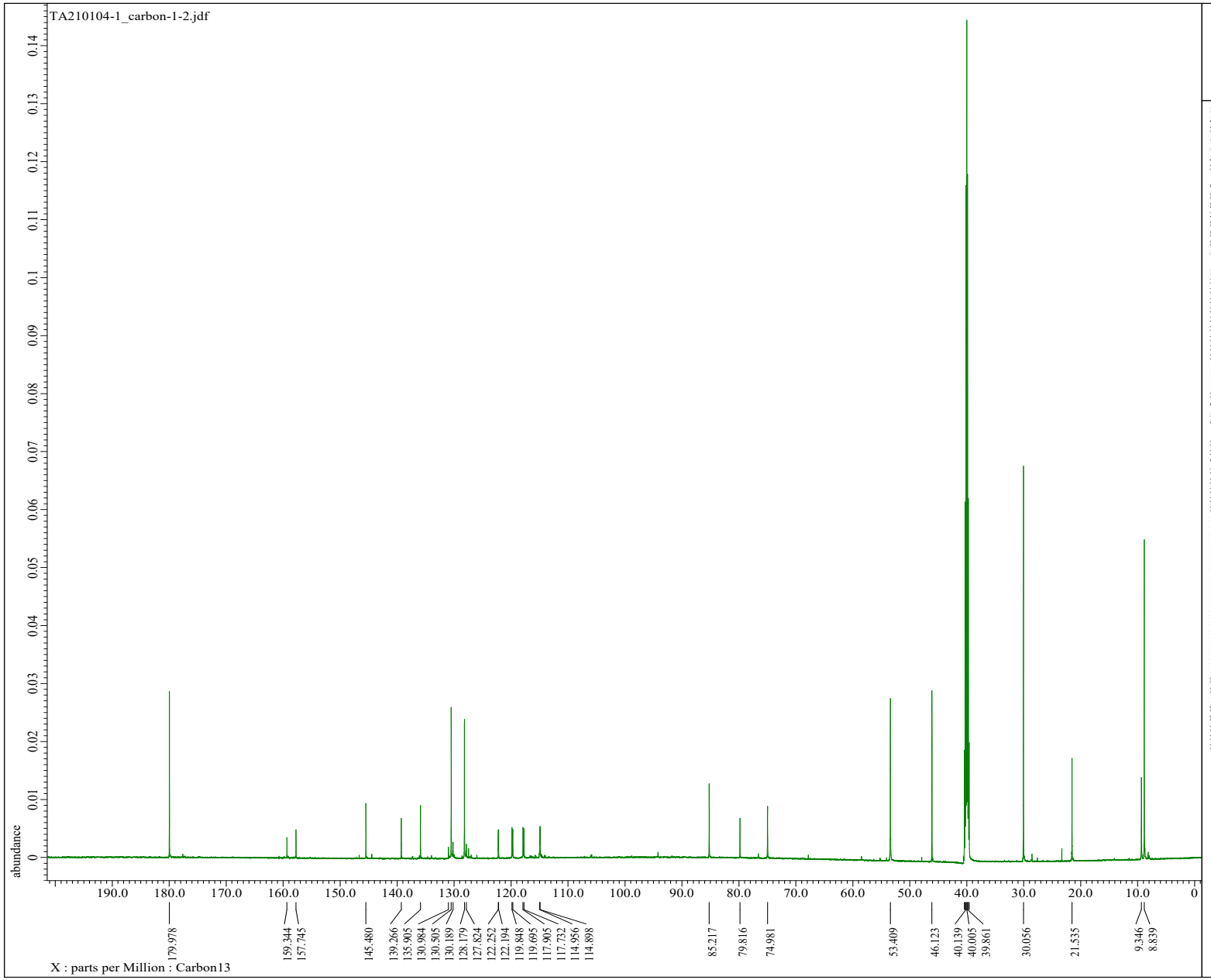

JEOL

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X_Offset	= 100[ppm]
X_Points	= 32768
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X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
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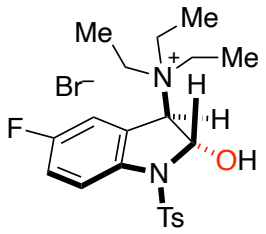

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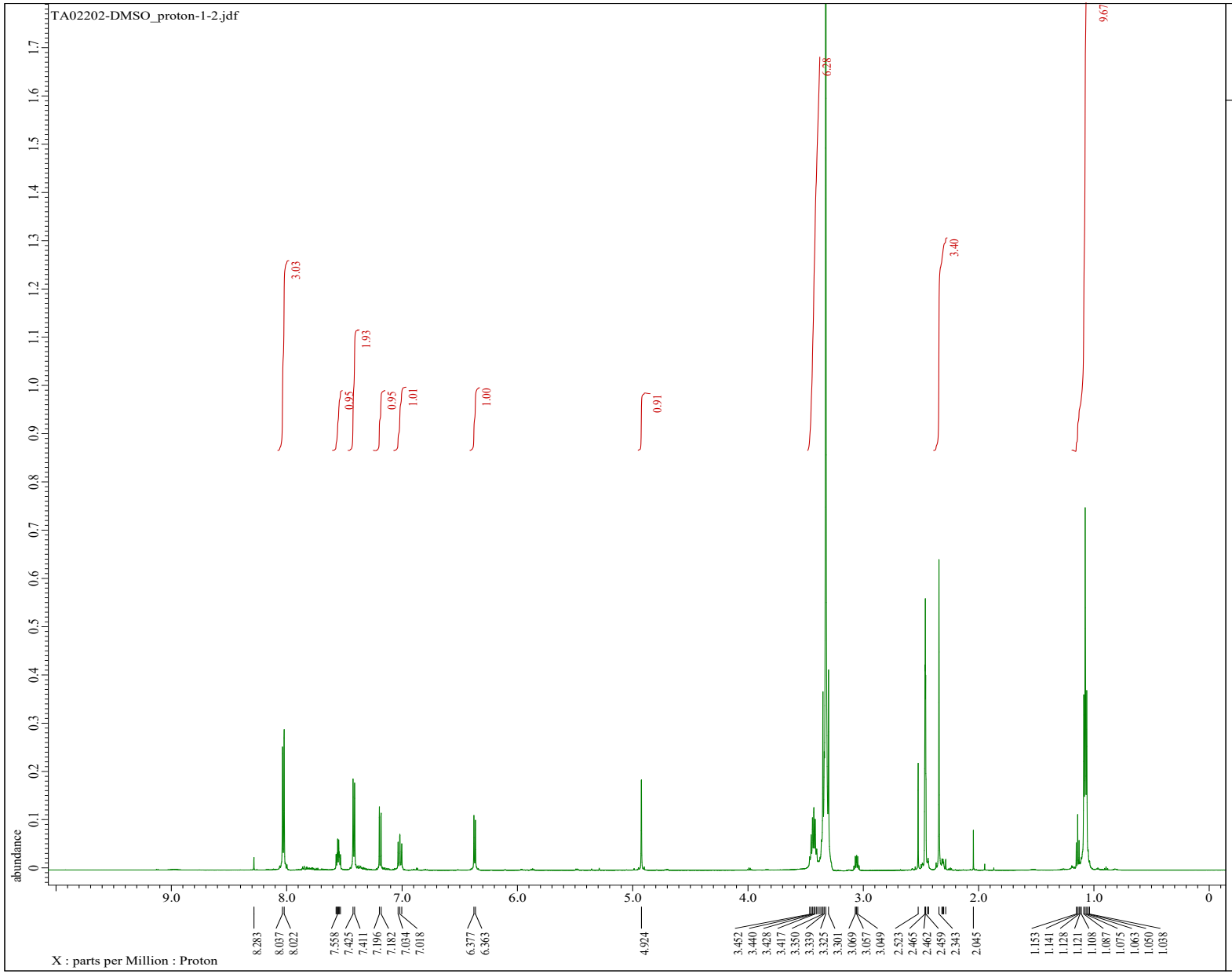

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Experiment	= proton.jxp
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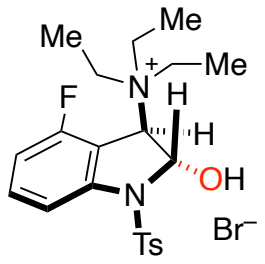

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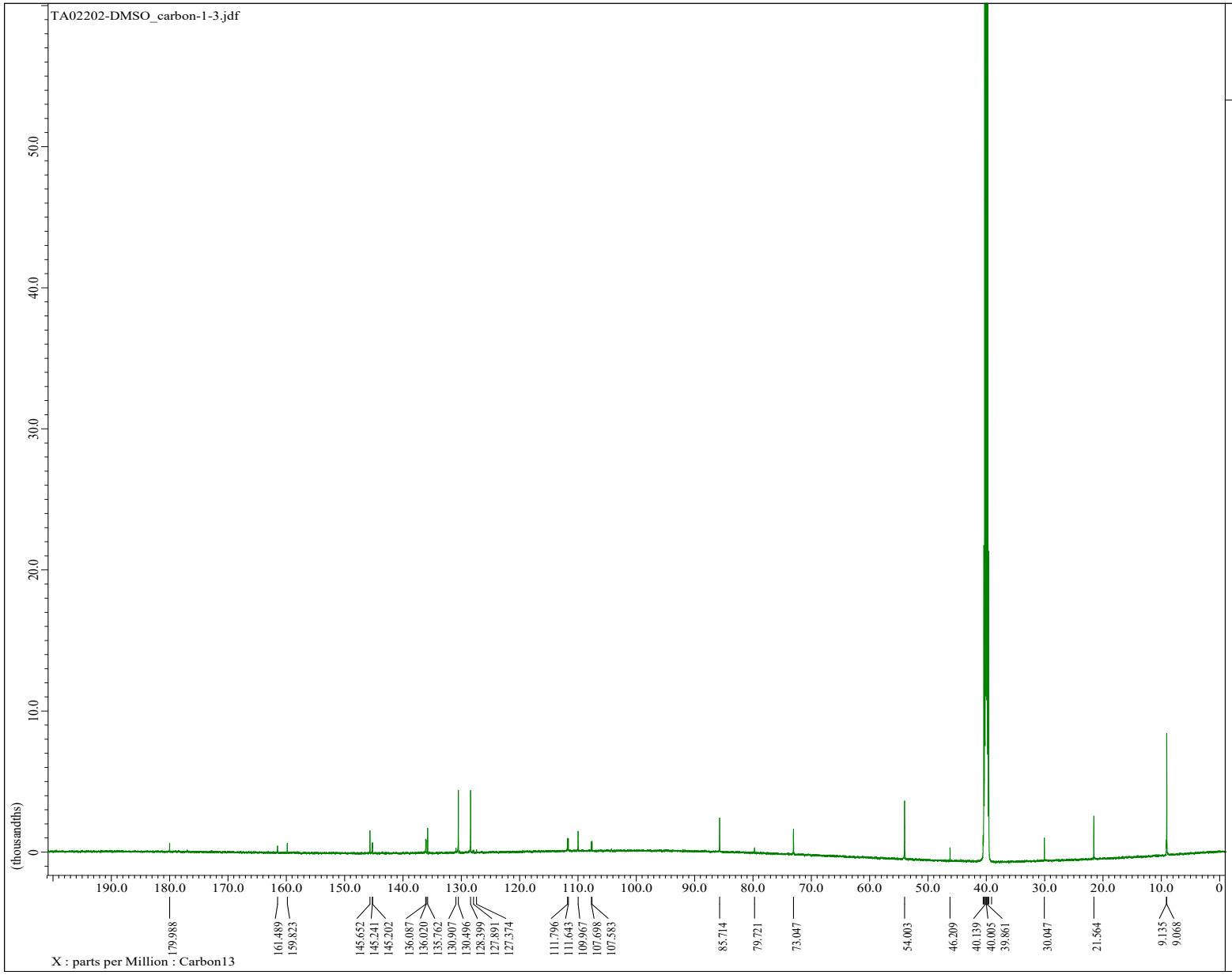

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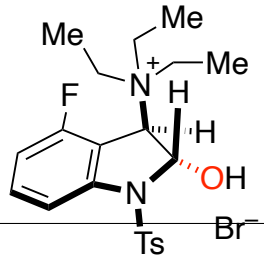

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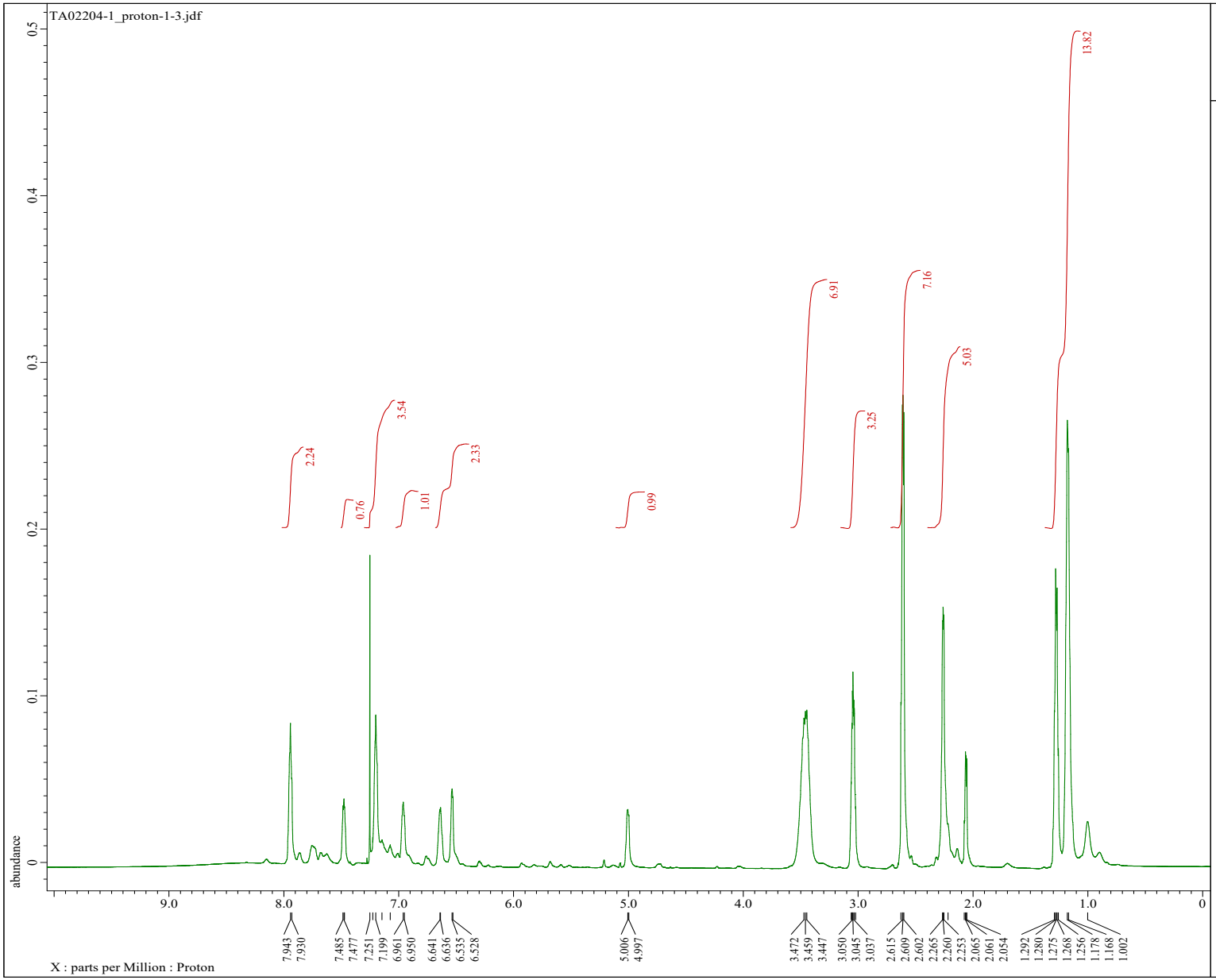

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X_Pulse	= 4.75[us]
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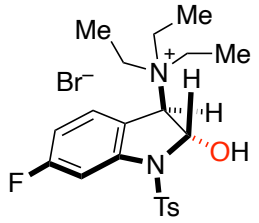

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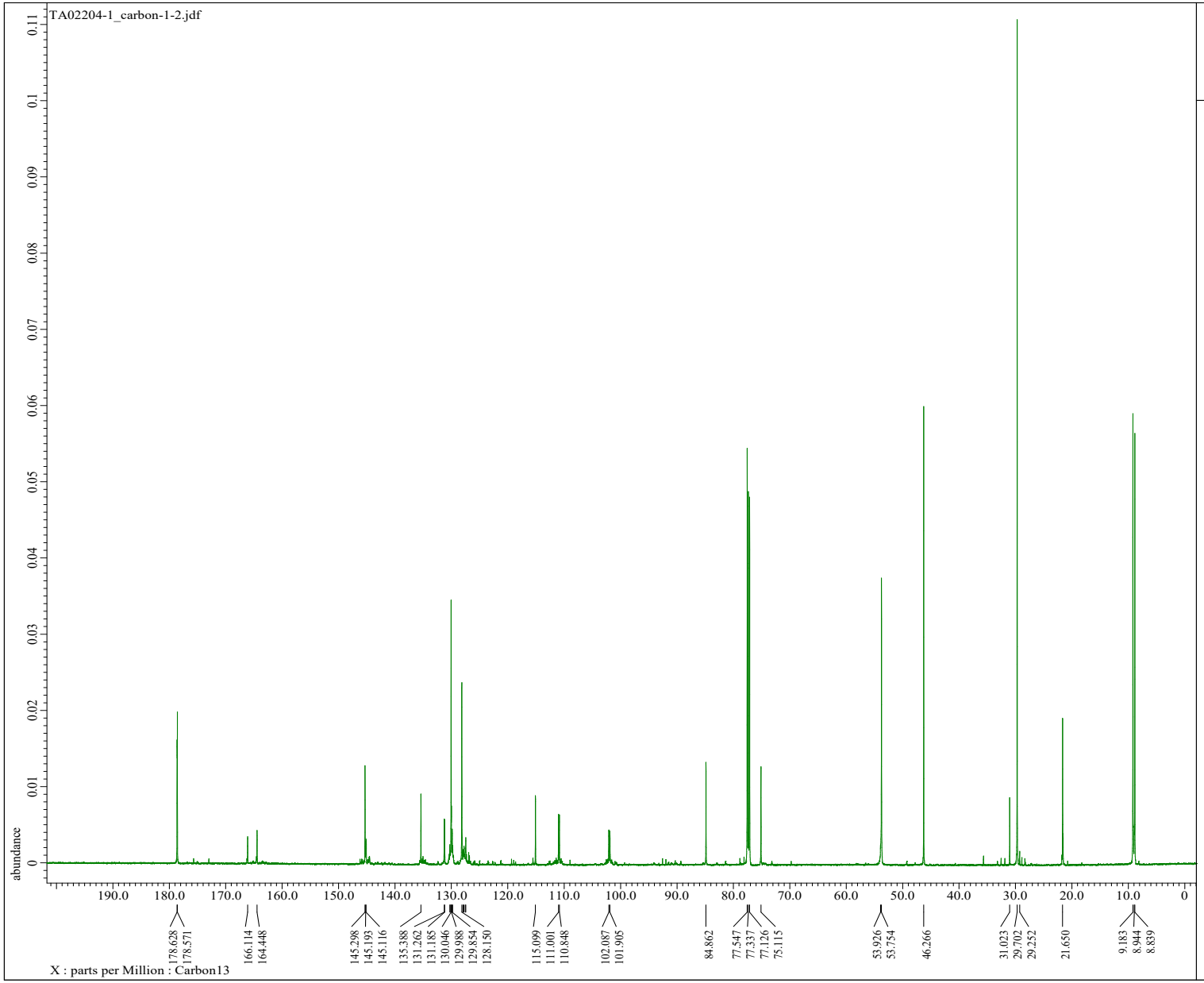

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X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
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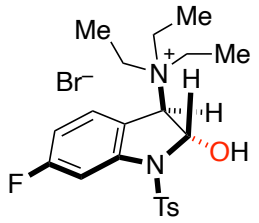
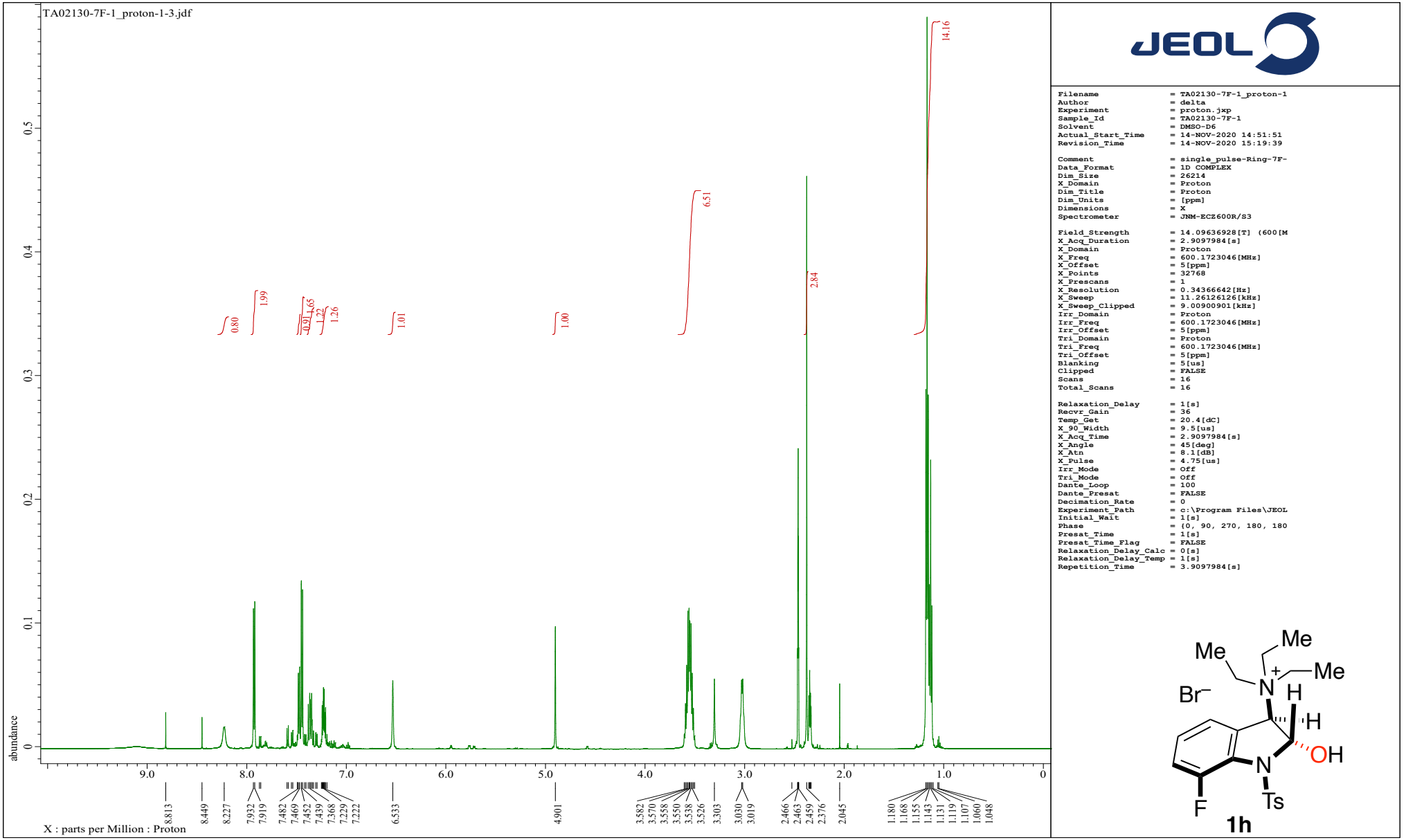
Repetition_Time	= 1.69206016[s]



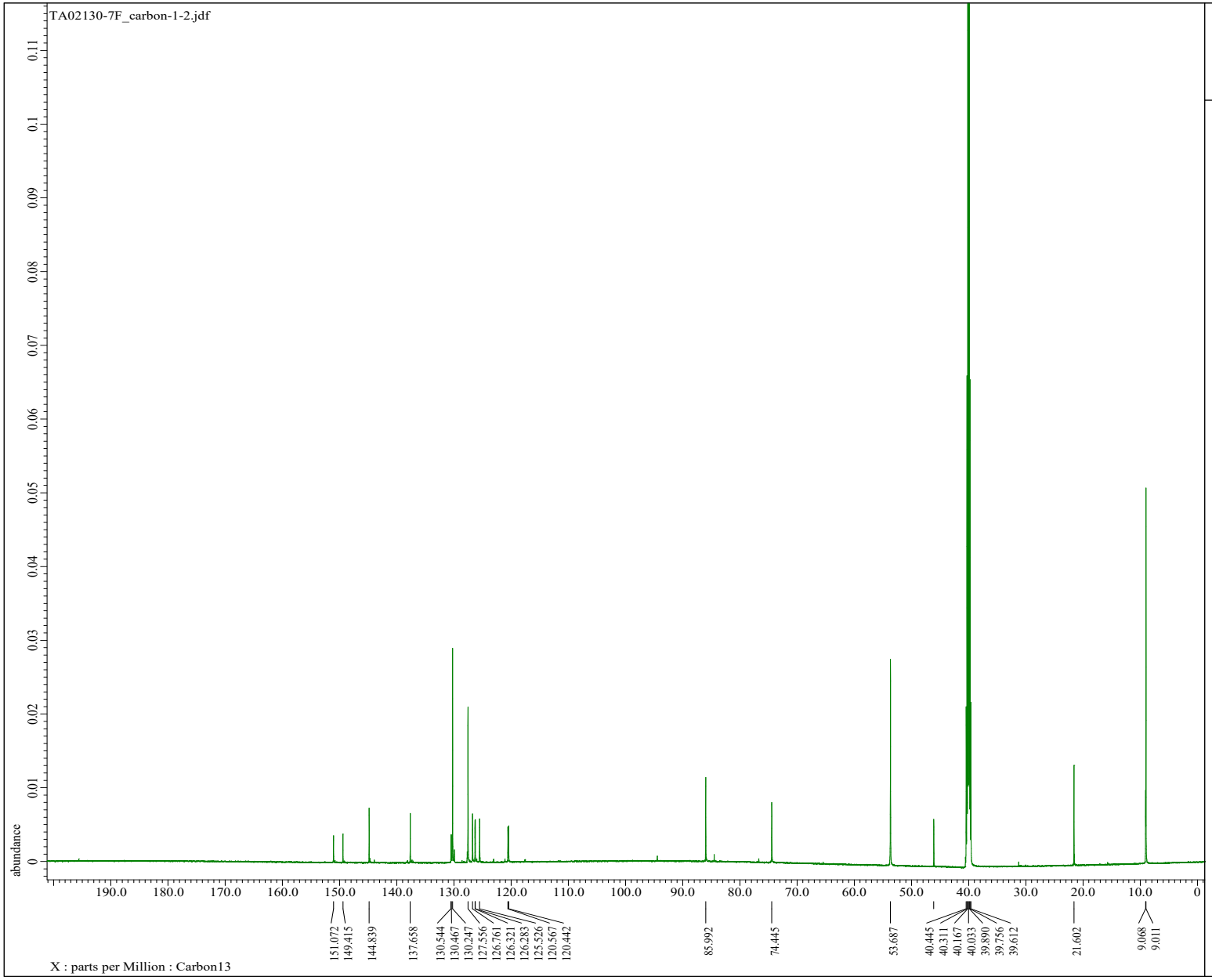
1g



JEOL

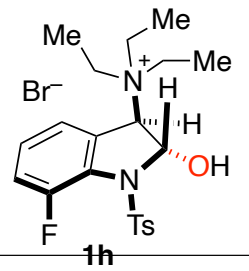
Filename	= TA02130-7F-1_proton-1
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA02130-7F-1
Solvent	= DMSO-D6
Actual_Start_Time	= 14-NOV-2020 14:51:51
Revision_Time	= 14-NOV-2020 15:19:39
Comment	= single_pulse-Ring-7F-
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.9097984[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.34366642[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 20.4[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 2.9097984[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	= 3.9097984[s]

1h

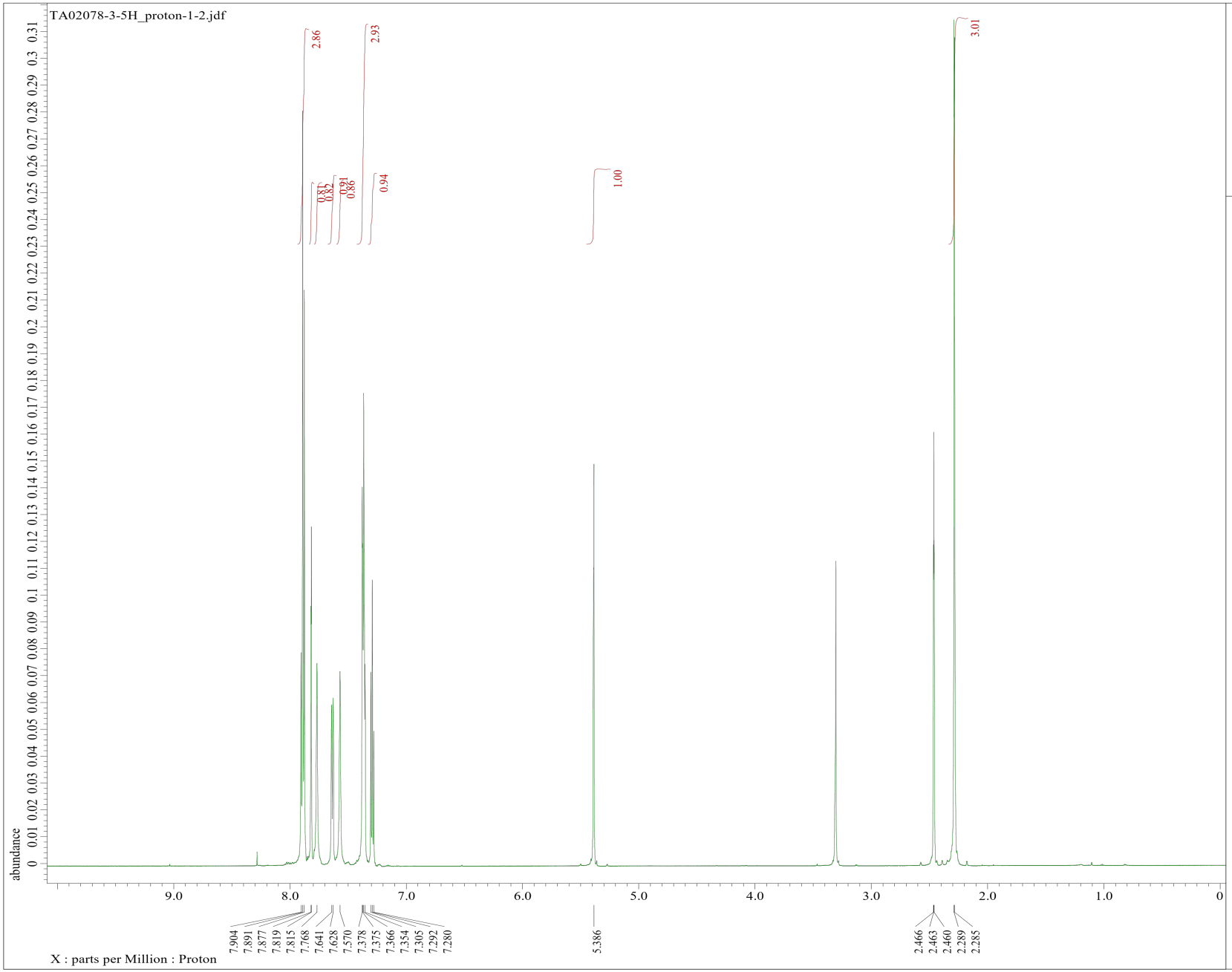


JEOL

Filename	= TA02130-7F_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA02130-7F
Solvent	= DMSO-D6
Actual_Start_Time	= 19-NOV-2020 20:22:
Revision_Time	= 19-NOV-2020 21:51:
Comment	= single pulse decou
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	= 2729
Total_Scans	= 2729
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.5[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_Templ	= 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]

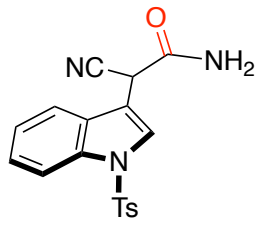


1h

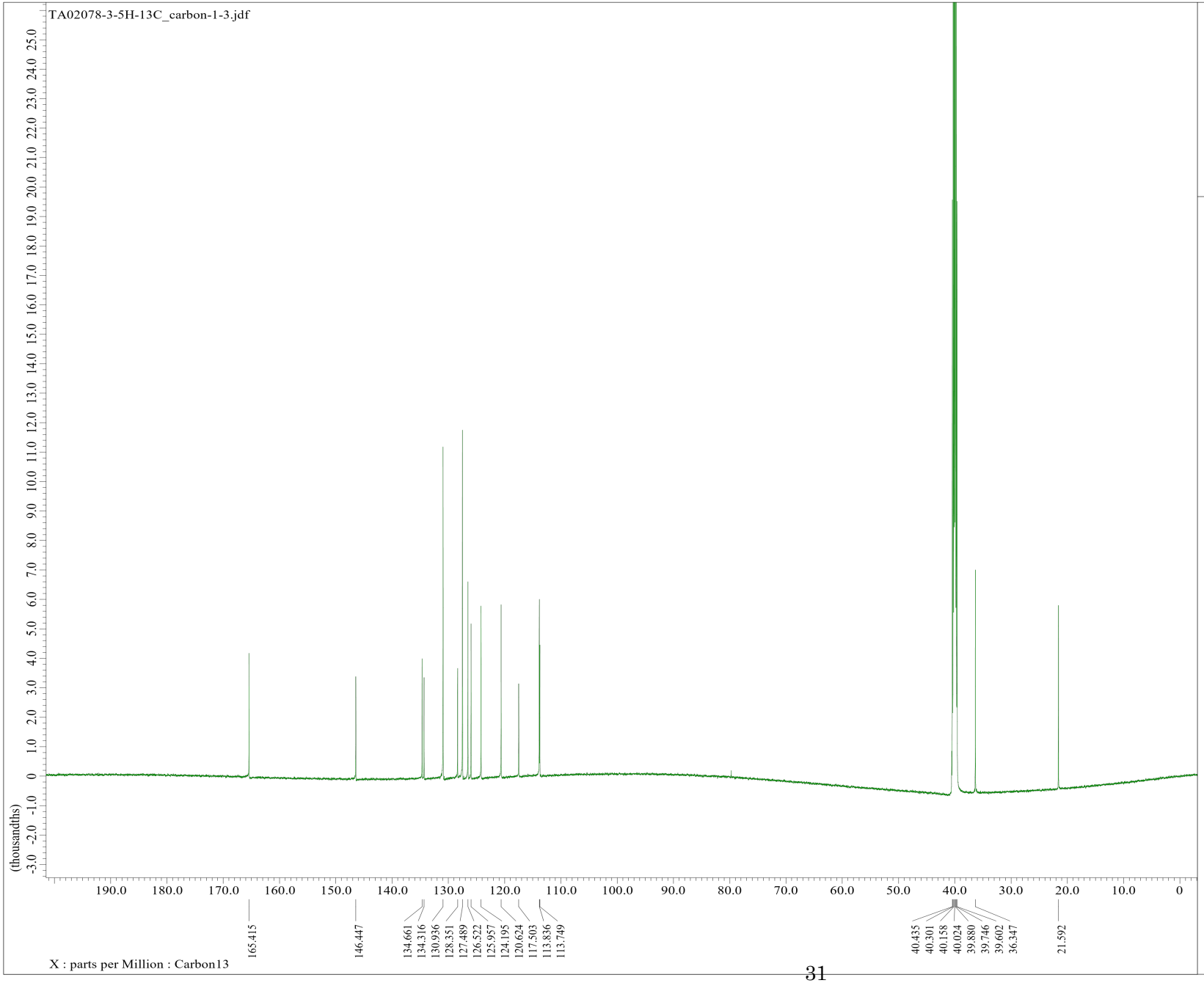



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: TA02078-3-5H_proton-1-1.jdf
```

Filename	= TA02078-3-5H_proton-1
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA02078-3-5H
Solvent	= DMSO-D6
Actual_Start_Time	= 6-NOV-2020 20:12:23
Revision_Time	= 6-NOV-2020 20:14:35
Comment	= single_pulse-5H
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	= 5[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 19.5[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 2.90455552[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	= 3.90455552[s]

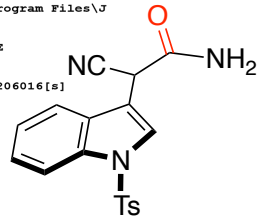


3aa

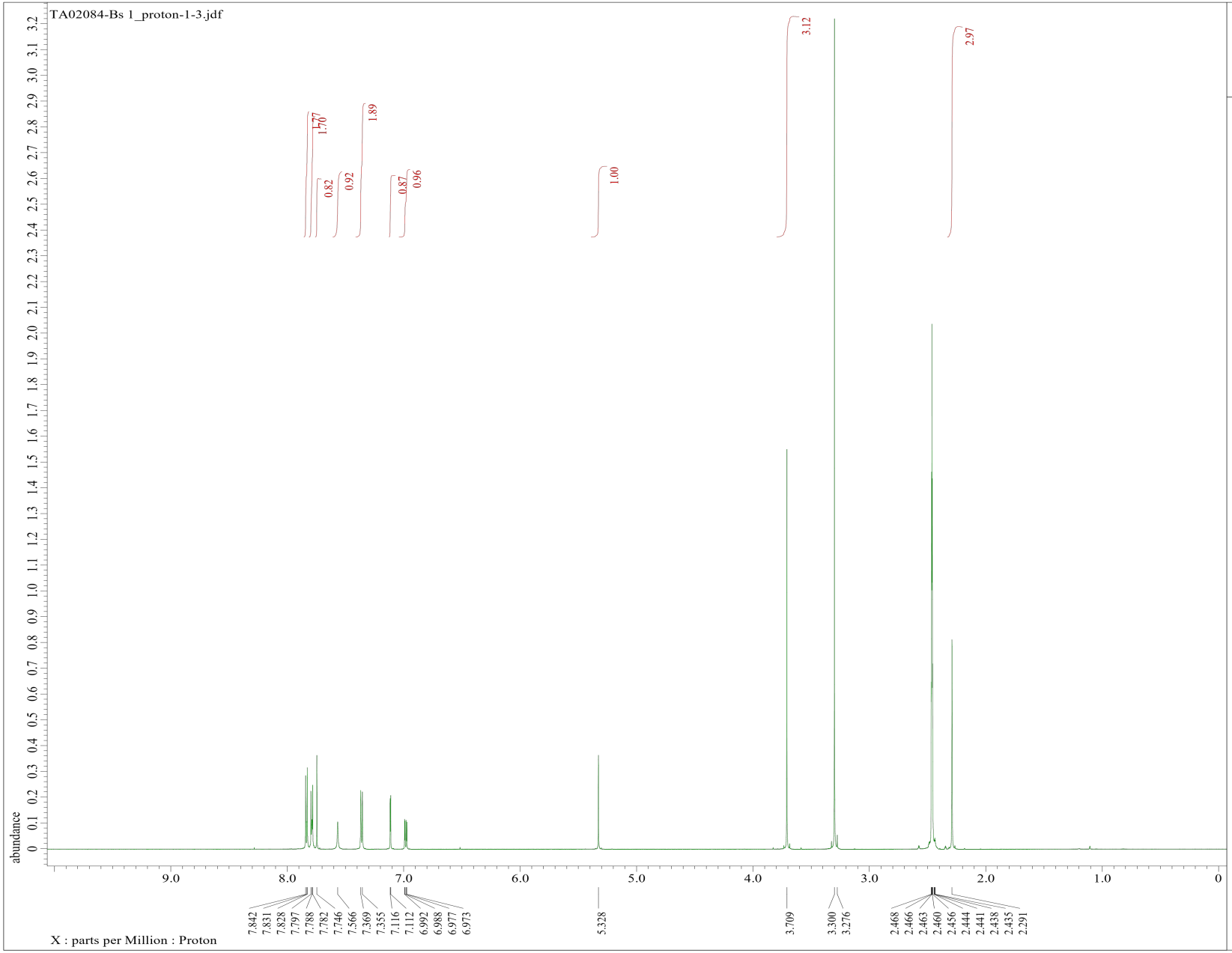



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: TA02078-3-5H-13C_carbon-1-1.jdf
```

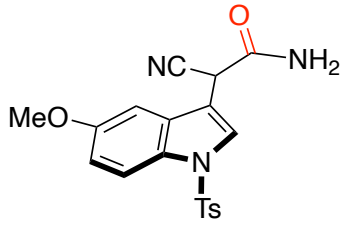
```
Filename                    = TA02078-3-5H-13C_c
Author                      = delta
Experiment                  = carbon.jxp
Sample_Id                   = TA02078-3-5H-13C
Solvent                     = DMSO-D6
Actual_Start_Time           =  7-NOV-2020 08:13:
Revision_Time               =  7-NOV-2020 12:45:

Comment                     = single pulse decou
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                       = 8167
Total_Scans                 = 8167

Relaxation_Delay            = 1[s]
Recvr_Gain                  = 56
Temp_Get                    = 20[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]
```



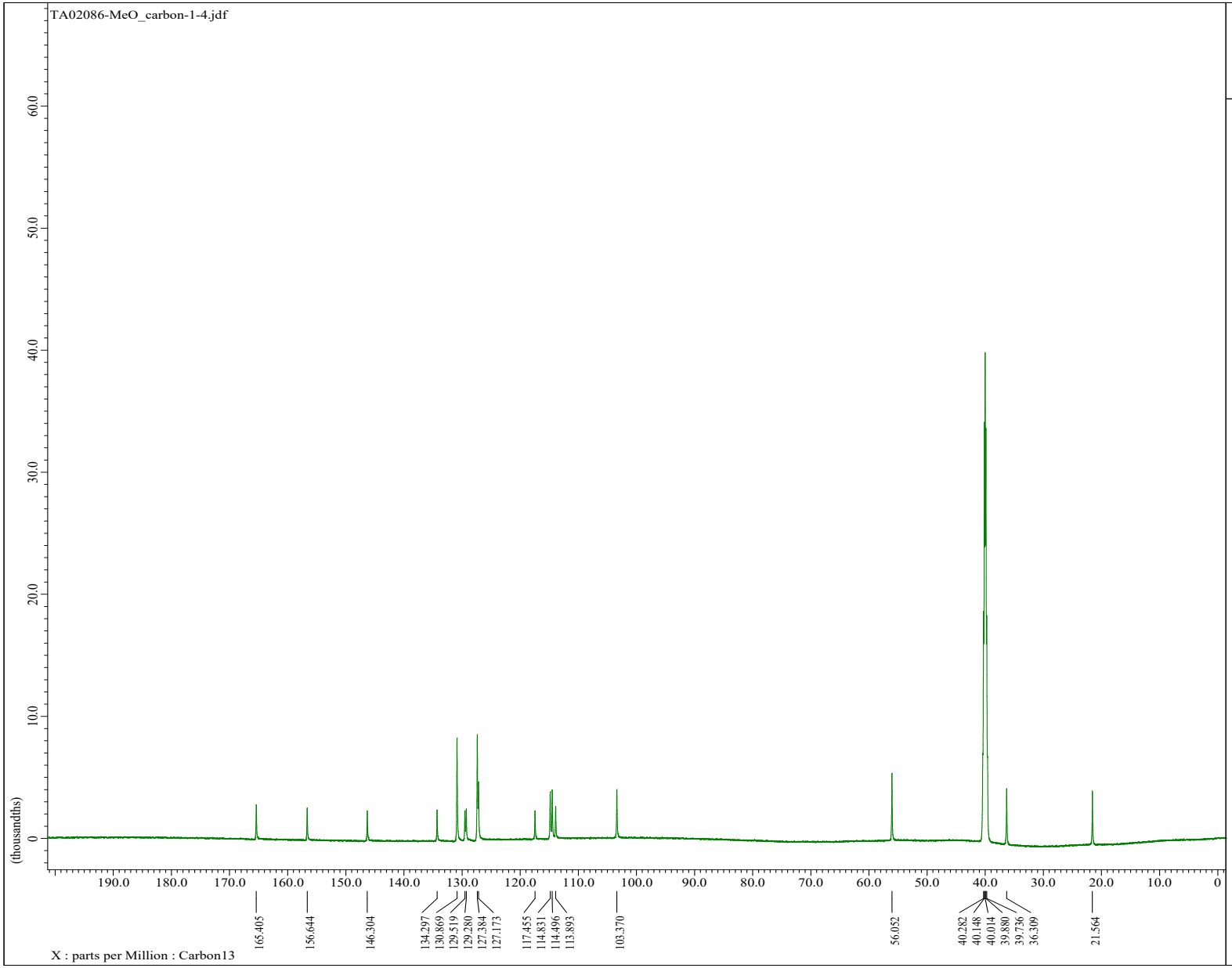
3aa



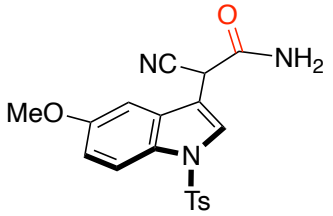

```
Filename                = TA02084-Bs 1_proton-1
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TA02084-Bs 1
Solvent                 = DMSO-D6
Actual_Start_Time       = 11-NOV-2020 08:43:52
Revision_Time           = 11-NOV-2020 08:55:37

Comment                 = single_pulse-Bs
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                = 5[us]
Clipped                 = TRUE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 1[s]
Recvr_Gain              = 56
Temp_Get                = 19.5[dC]
X_90_Width              = 9.5[us]
X_Acq_Time              = 2.90455552[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         = 3.90455552[s]
```



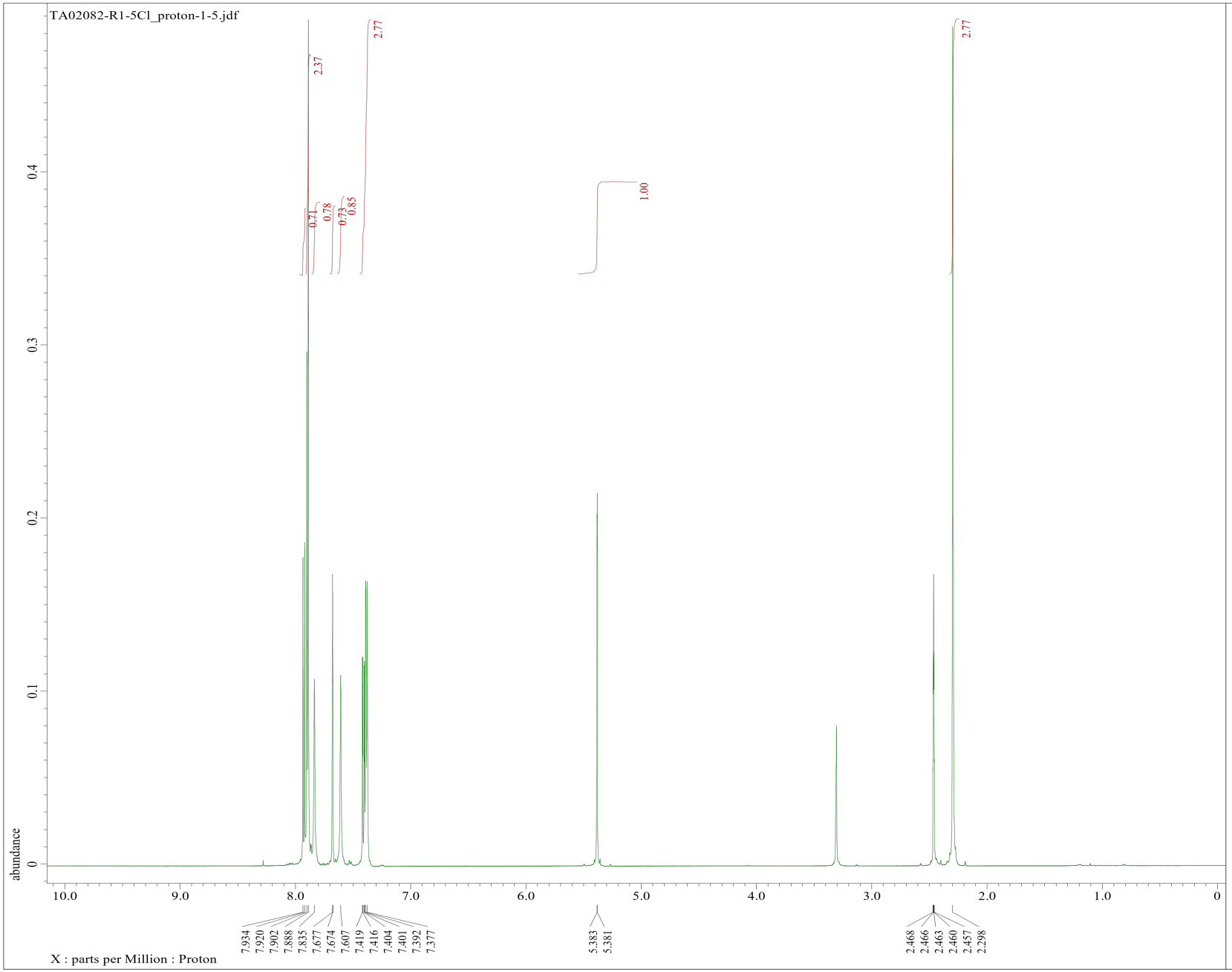
3ba



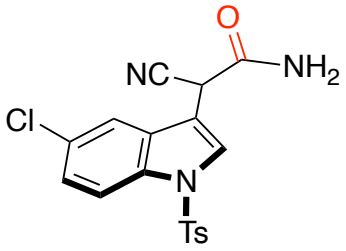
Filename	= TA02086-MeO_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA02086-MeO
Solvent	= DMSO-D6
Actual_Start_Time	= 10-NOV-2020 21:13:
Revision_Time	= 18-JAN-2021 08:07:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [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	= 5000
Total_Scans	= 5000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 19.8[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_Templ	= 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]



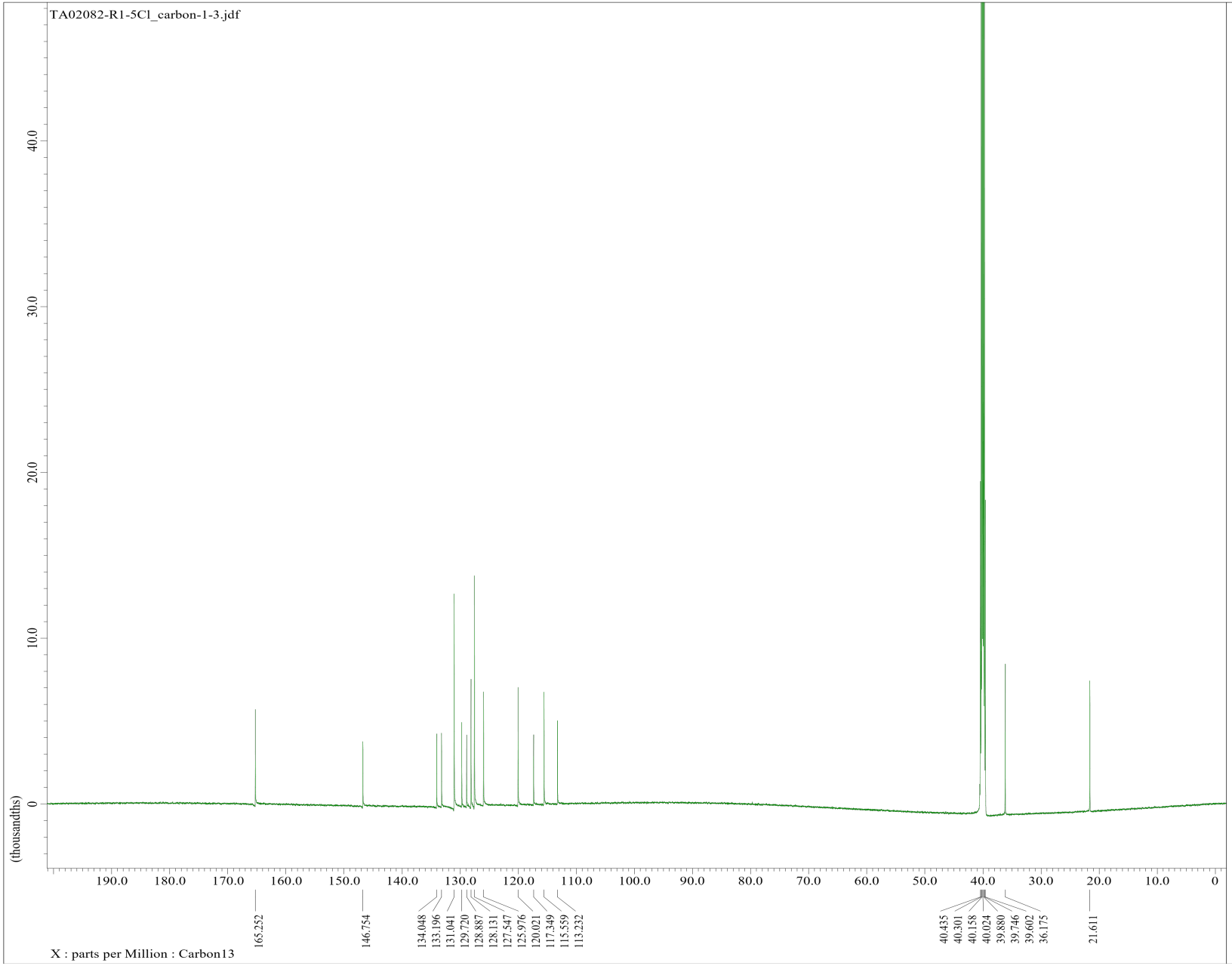
3ba



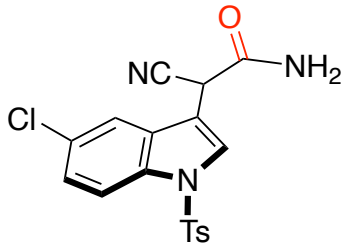
Filename	= TA02082-R1-5Cl_proton
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA02082-R1-5Cl
Solvent	= DMSO-D6
Actual_Start_Time	= 7-NOV-2020 16:00:41
Revision_Time	= 7-NOV-2020 16:17:58
Comment	= single_pulse-5Cl-5H
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
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	= 5[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 20.3[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 2.90455552[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	= 3.90455552[s]



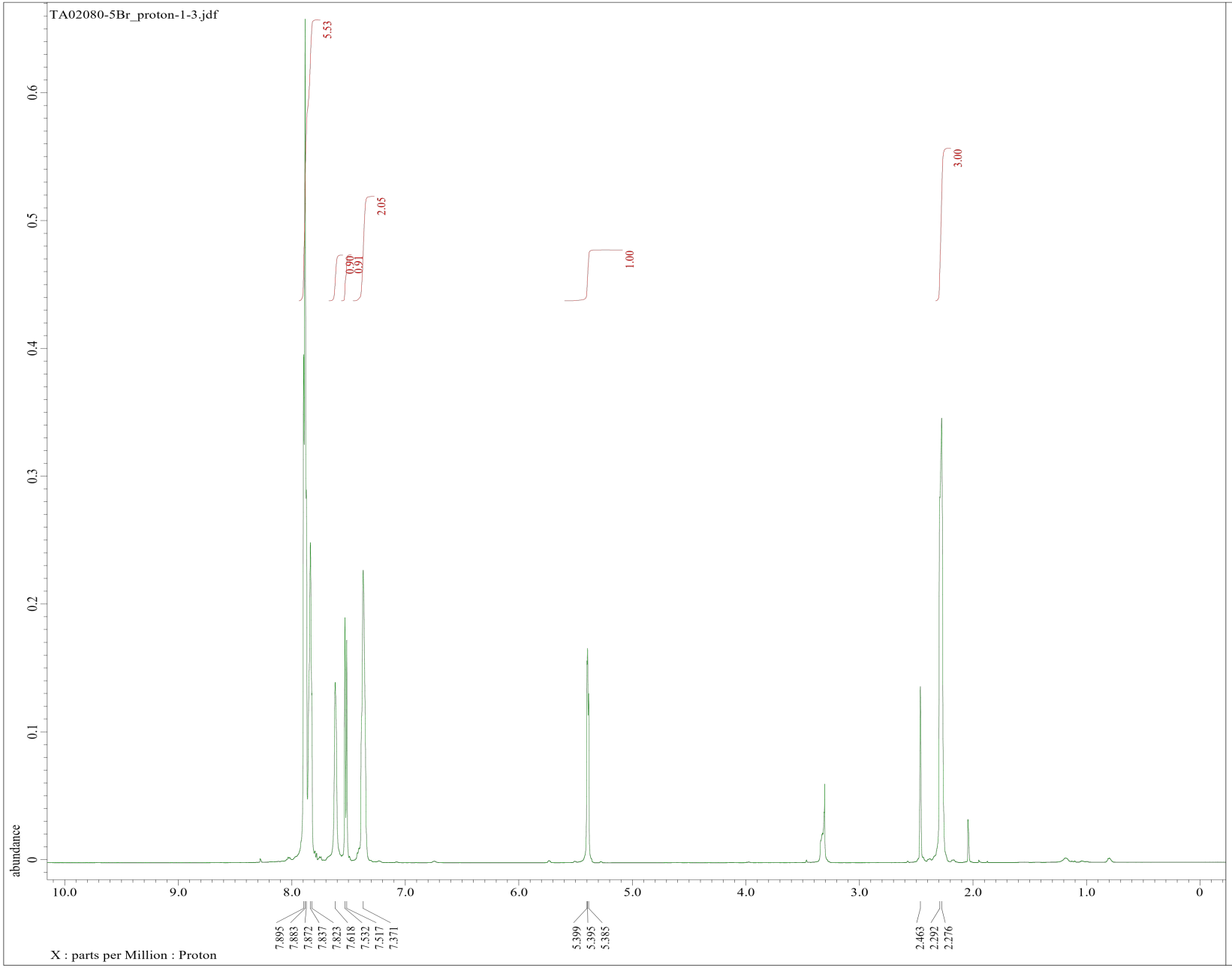
3ca



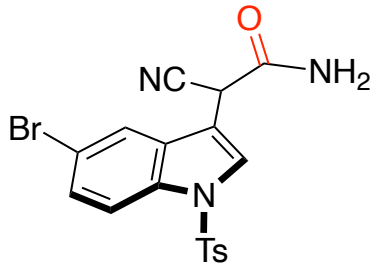

```
Filename                  = TA02082-R1-5Cl_car
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = TA02082-R1-5Cl
Solvent                   = DMSO-D6
Actual_Start_Time         =  7-NOV-2020 16:09:
Revision_Time             =  7-NOV-2020 18:33:

Comment                   = single pulse decou
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                     = 4213
Total_Scans               = 4213

Relaxation_Delay          = 1[s]
Recvr_Gain                = 56
Temp_Get                  = 19.7[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]
```



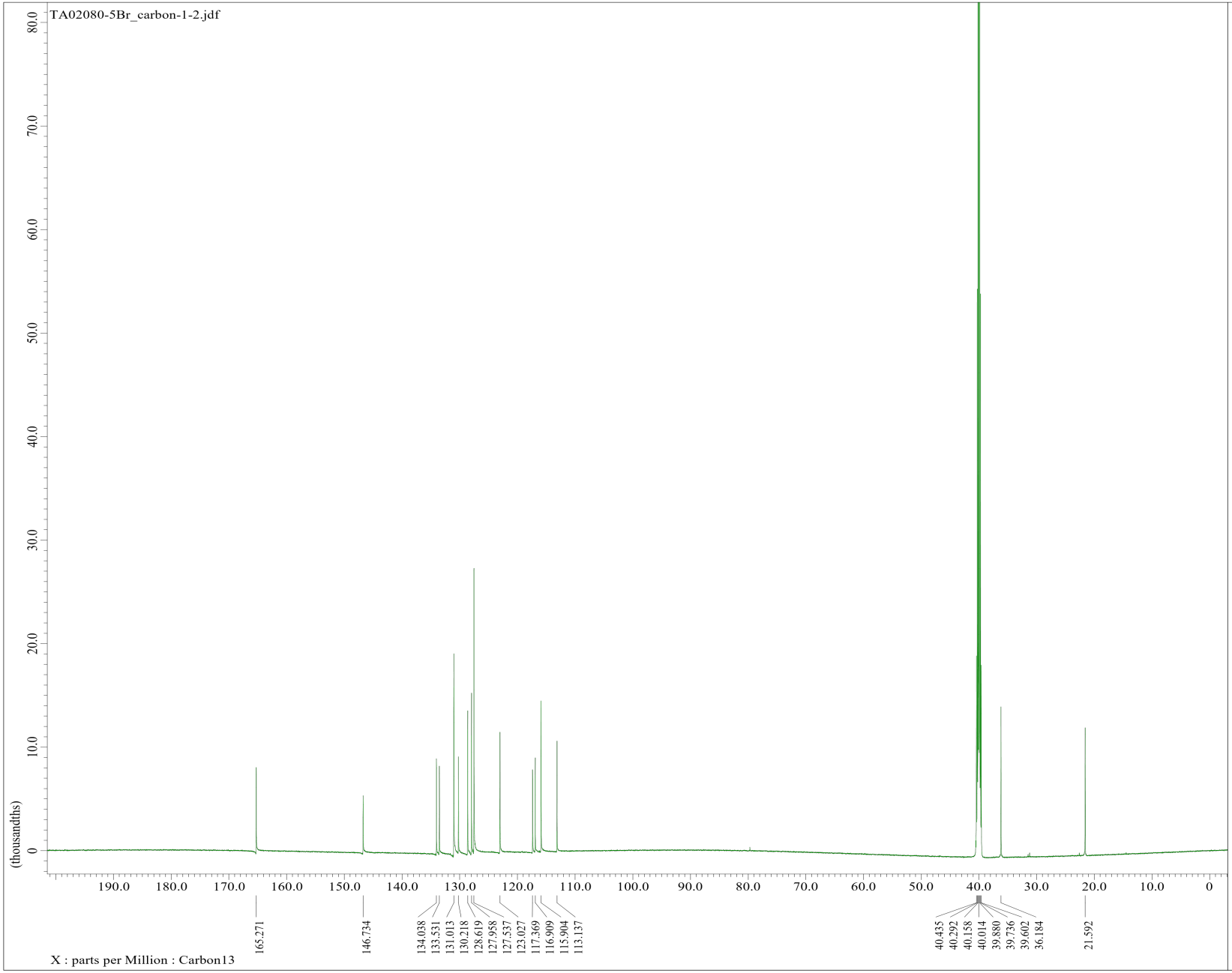
3ca



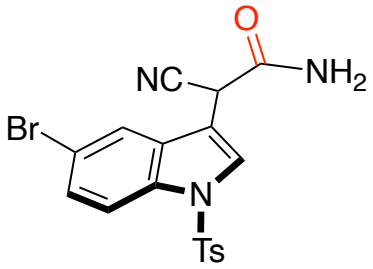

```
Filename                = TA02080-5Br_proton-1-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TA02080-5Br
Solvent                 = DMSO-D6
Actual_Start_Time       =  7-NOV-2020 16:04:50
Revision_Time           =  7-NOV-2020 16:14:59

Comment                 = single_pulse-5Br-5H
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                = 5[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 1[s]
Recvr_Gain              = 36
Temp_Get                = 20.8[dC]
X_90_Width              = 9.5[us]
X_Acq_Time              = 2.90455552[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         = 3.90455552[s]
```



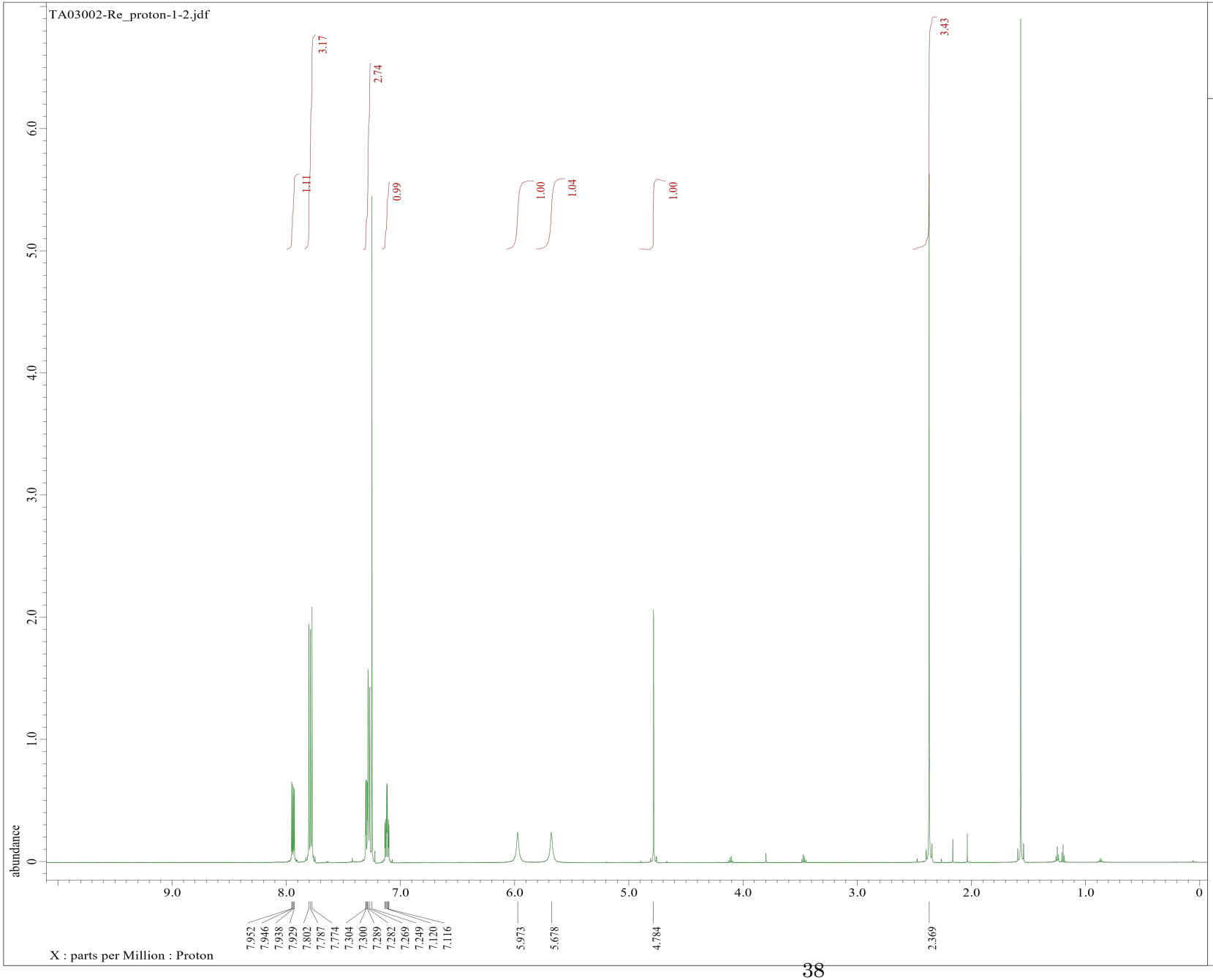
3da



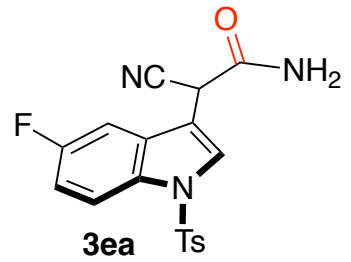

```
Filename                  = TA02080-5Br_carbon
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = TA02080-5Br
Solvent                   = DMSO-D6
Actual_Start_Time         =  7-NOV-2020 18:34:
Revision_Time             =  8-NOV-2020 09:21:

Comment                   = single pulse decou
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                     = 7000
Total_Scans               = 7000

Relaxation_Delay          = 1[s]
Recvr_Gain                = 56
Temp_Get                  = 19.8[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]
```



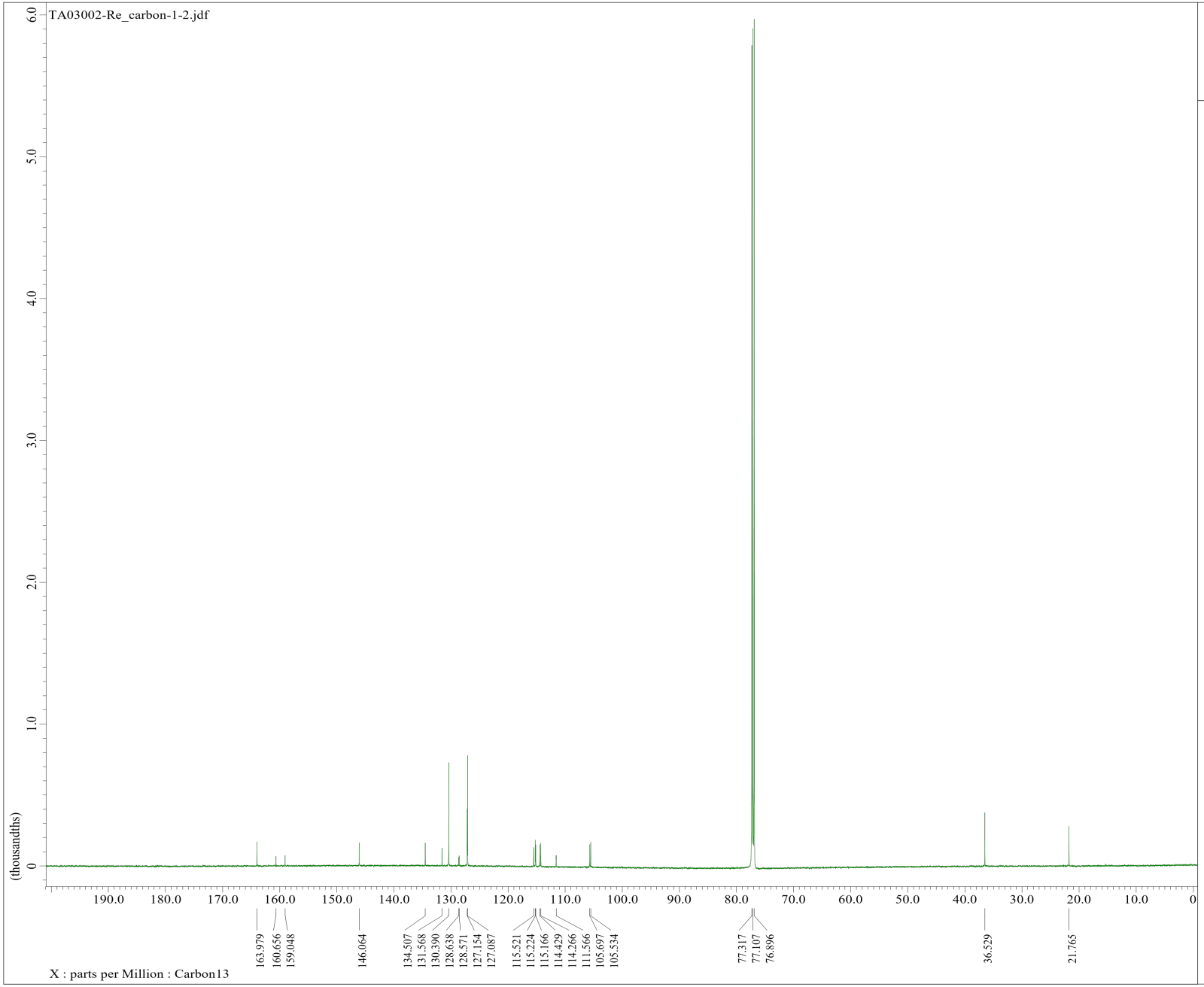
3da



Filename	= TA03002-Re_proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA03002-Re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-JAN-2021 05:32:21
Revision_Time	= 6-JAN-2021 08:14:08
Comment	= single_pulse-5F-indol
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.7[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]

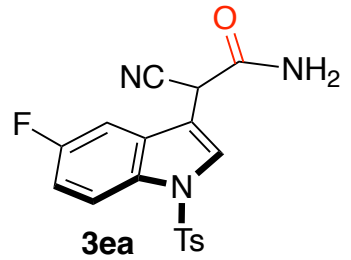


3ea

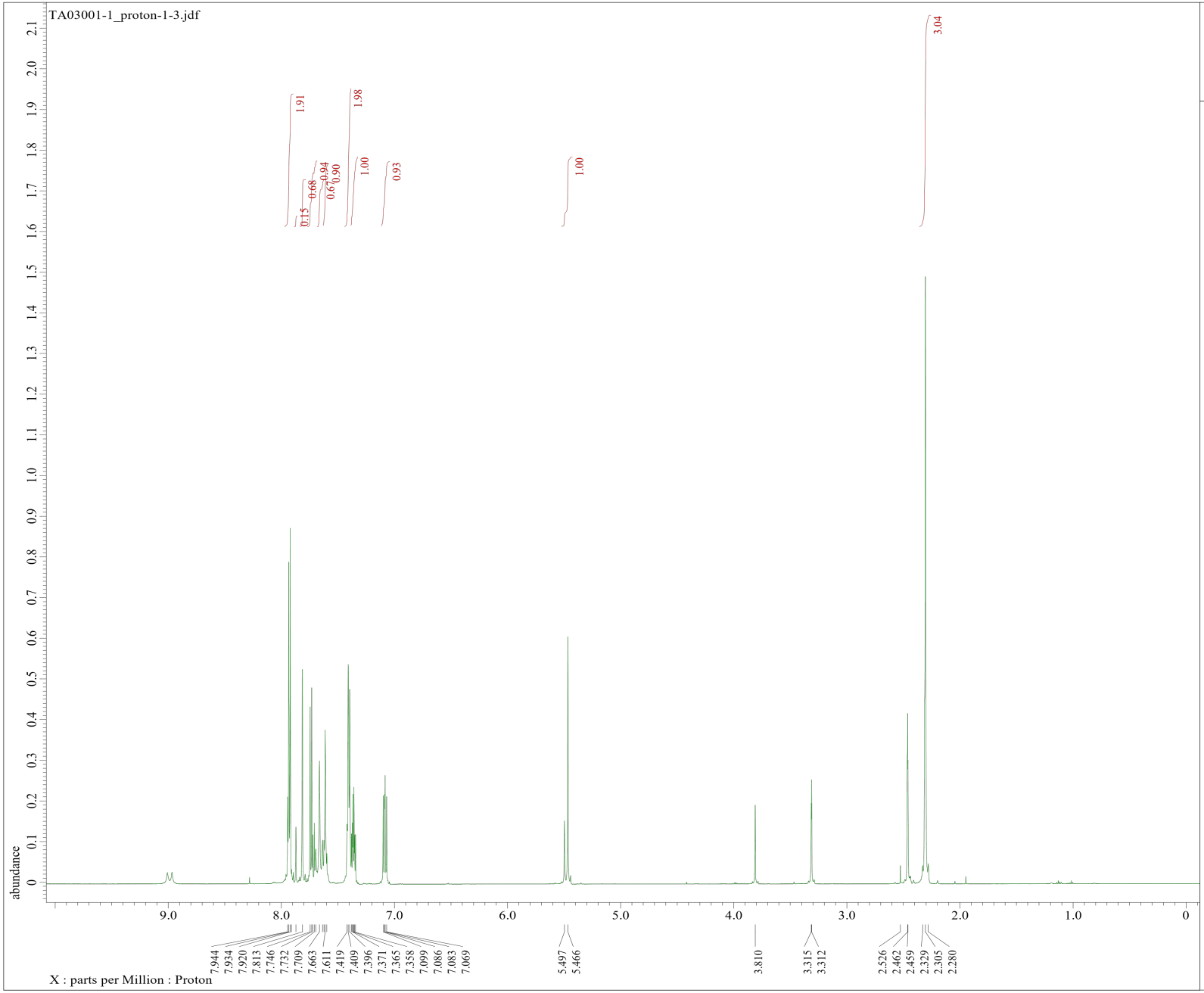


JEOL

Filename	= TA03002-Re_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA03002-Re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-JAN-2021 05:37:
Revision_Time	= 6-JAN-2021 08:14:
Comment	= single pulse decou
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	= 4785
Total_Scans	= 4785
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 19.8[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]

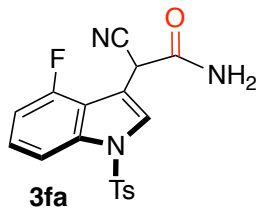


3ea

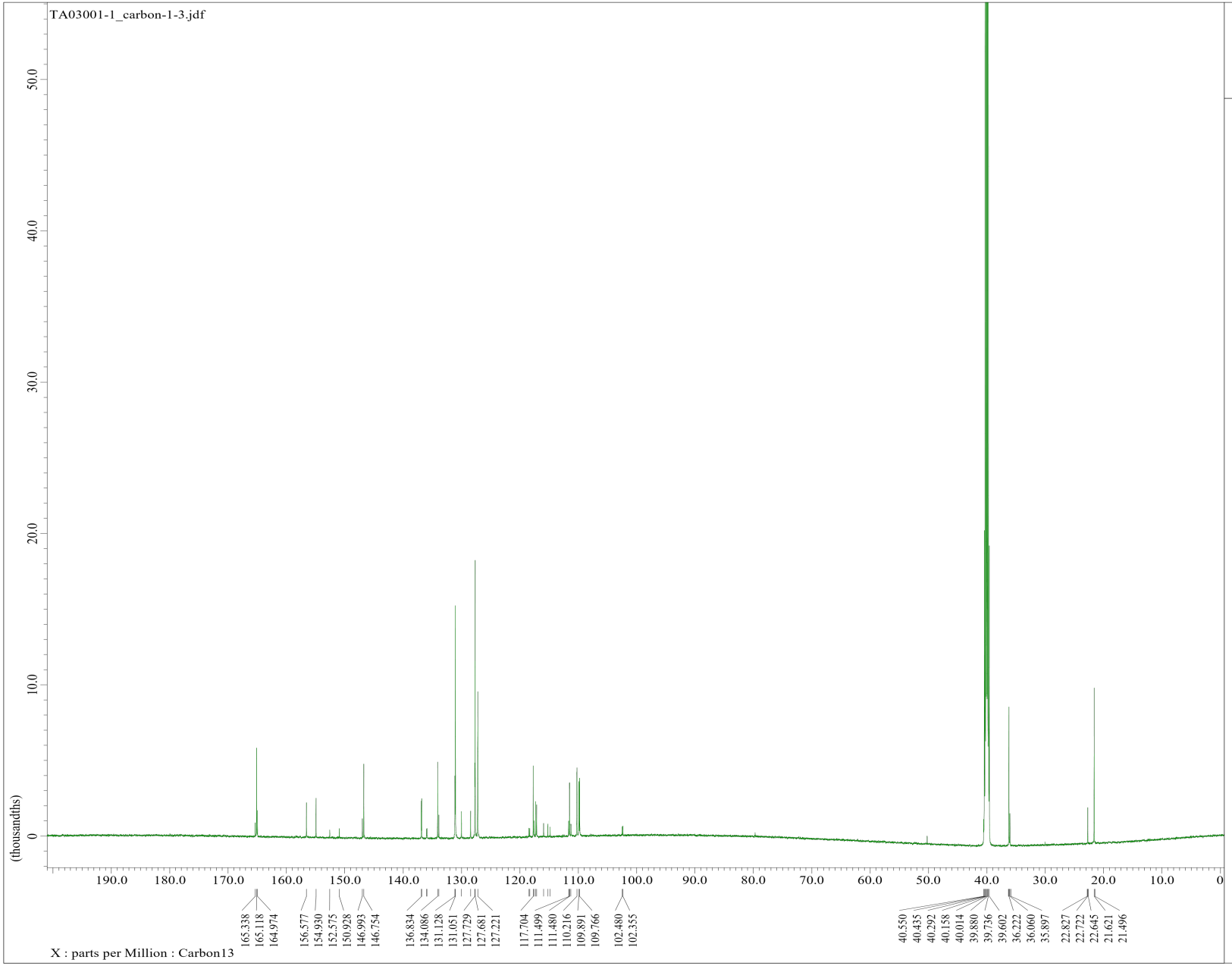


JEOL

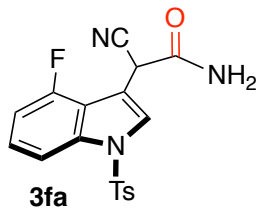
Filename	= TA03001-1_proton-1-3.
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA03001-1
Solvent	= DMSO-D6
Actual_Start_Time	= 22-DEC-2020 20:21:57
Revision_Time	= 22-DEC-2020 20:29:50
Comment	= single_pulse-4F-indol
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.09051904[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.91699454[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	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 19.6[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.09051904[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.09051904[s]



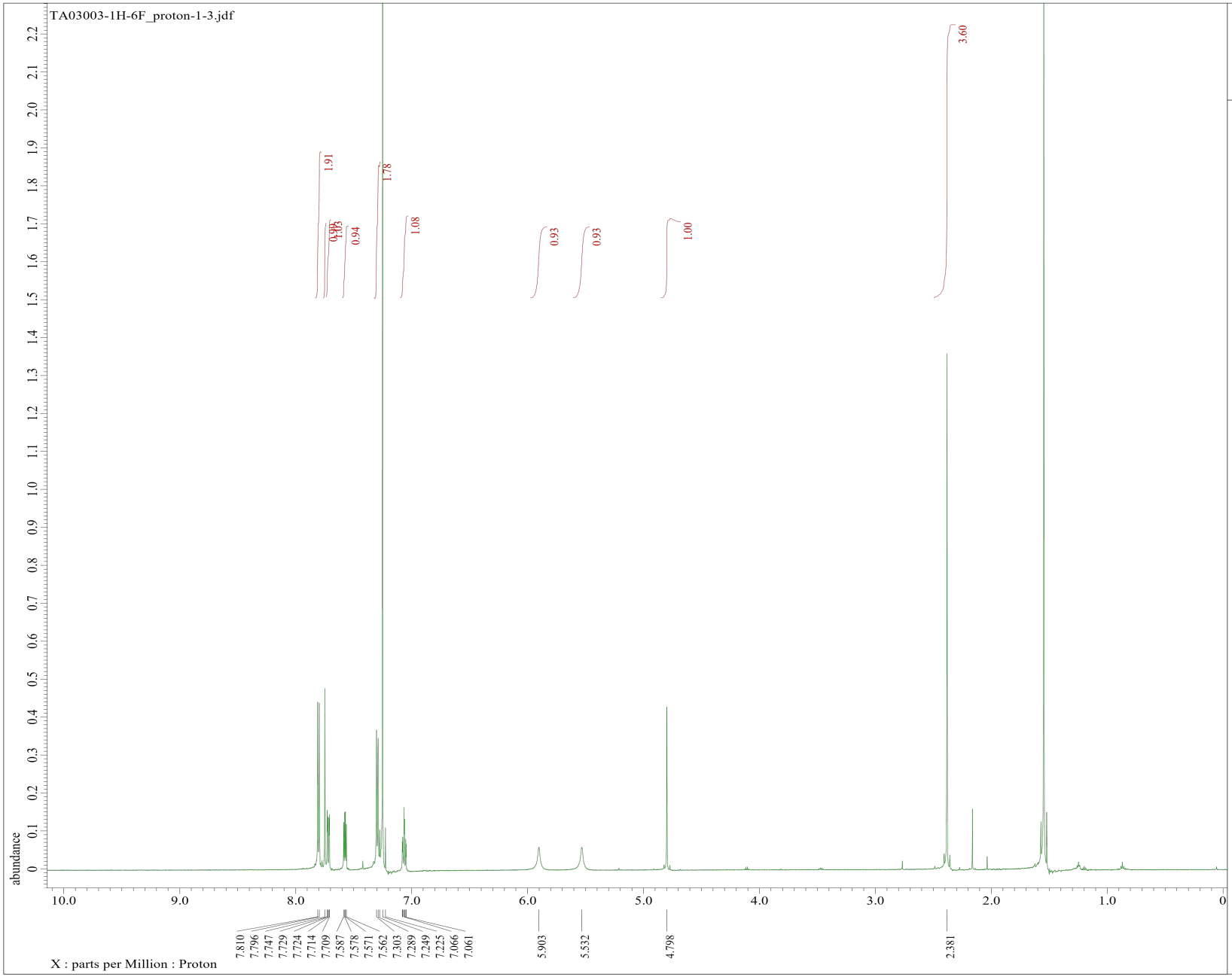
3fa



Filename	= TA03001-1_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA03001-1
Solvent	= DMSO-D6
Actual_Start_Time	= 22-DEC-2020 20:26:
Revision_Time	= 22-DEC-2020 22:24:
Comment	= single pulse decou
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	= 3000
Total_Scans	= 3000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 19.6[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]

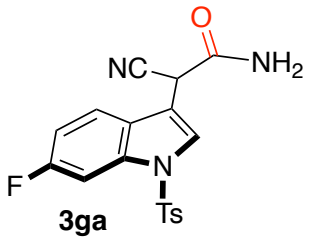


3fa

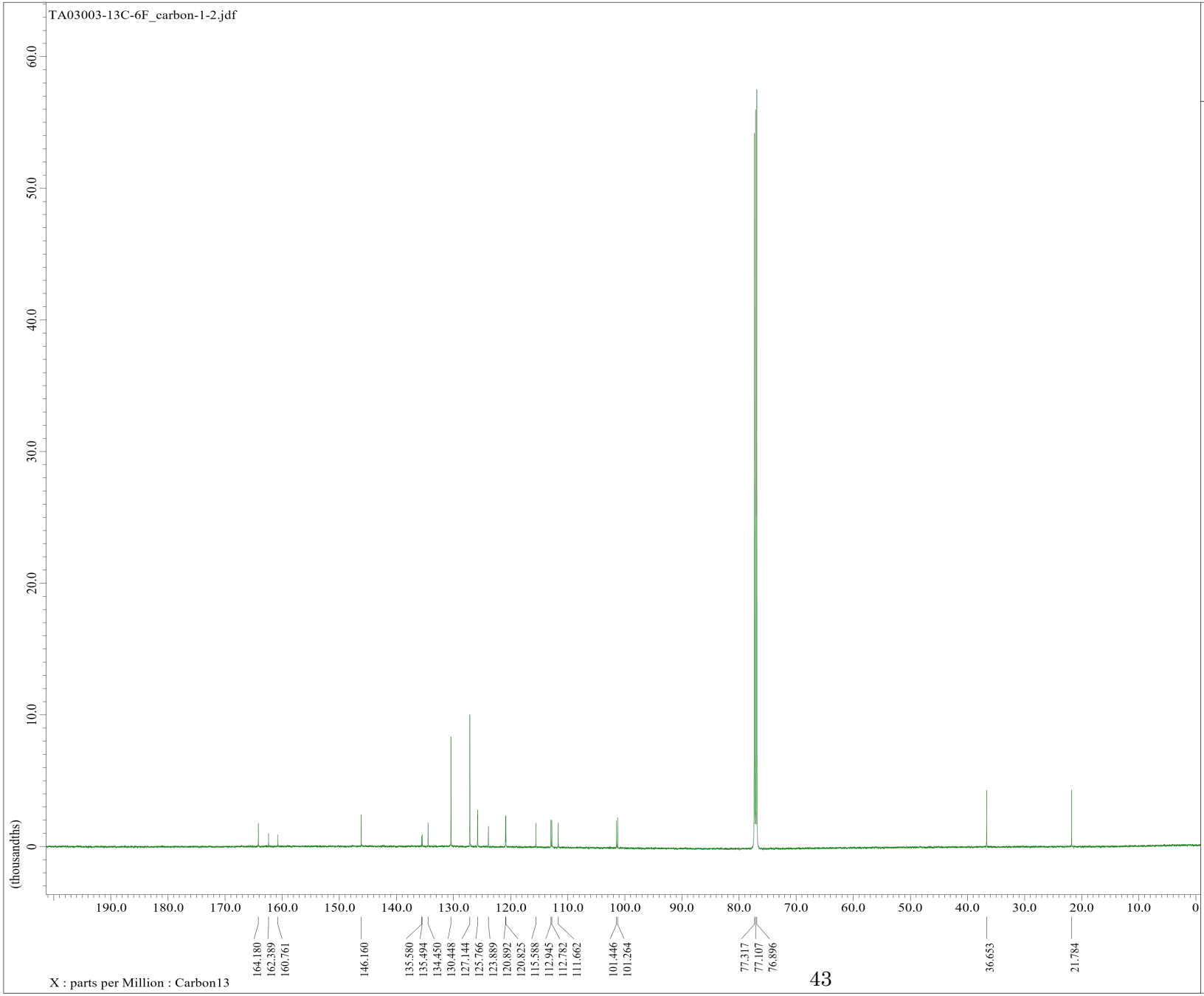


JEOL

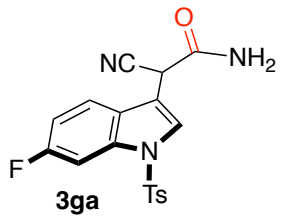
Filename	= TA03003-1H-6F_proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA03003-1H-6F
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-DEC-2020 20:18:08
Revision_Time	= 21-DEC-2020 20:25:13
Comment	= single_pulse-6F-indol
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.09051904[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.91699454[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	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.8[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.09051904[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.09051904[s]



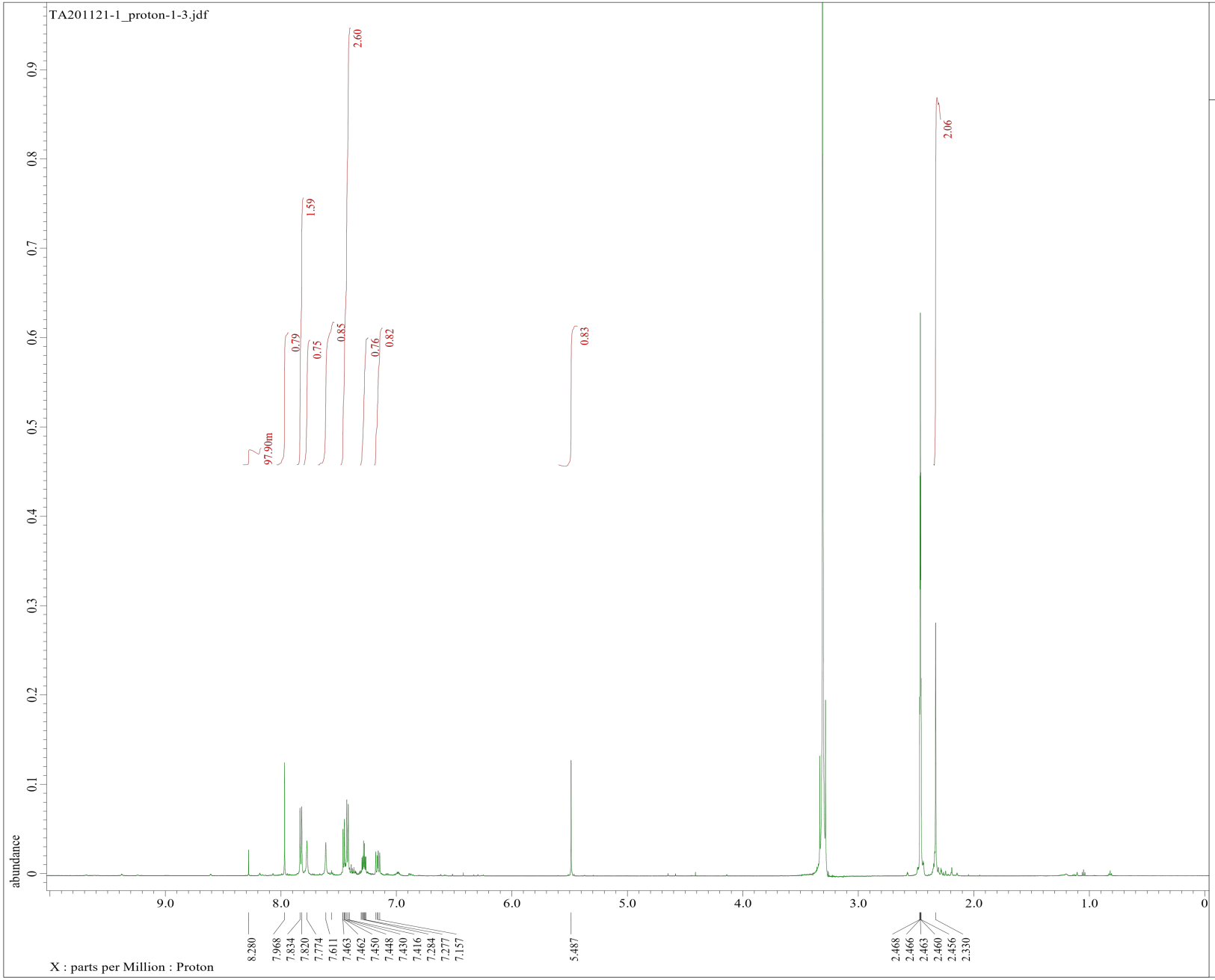
3ga



Filename	= TA03003-13C-6F_car
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA03003-13C-6F
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-DEC-2020 20:31:
Revision_Time	= 21-DEC-2020 22:10:
Comment	= single pulse decou
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	= 3000
Total_Scans	= 3000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
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]

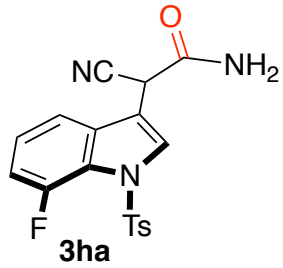


3ga

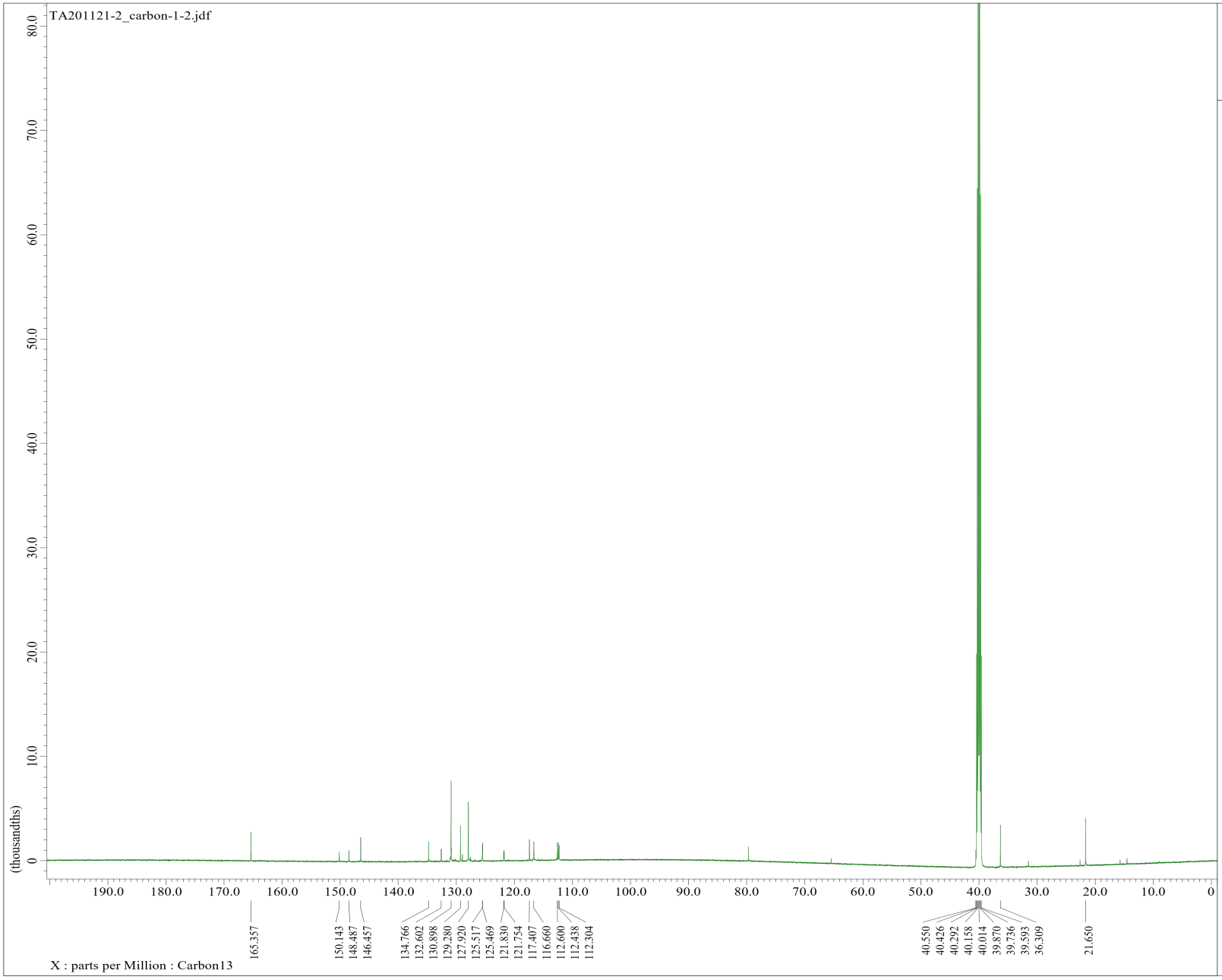


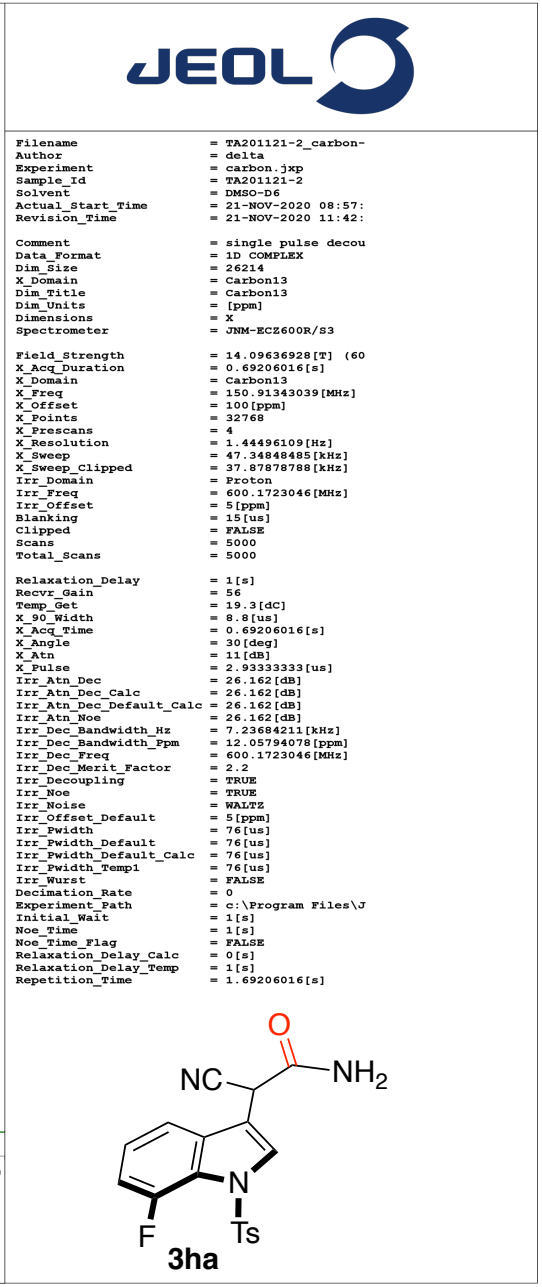
JEOL

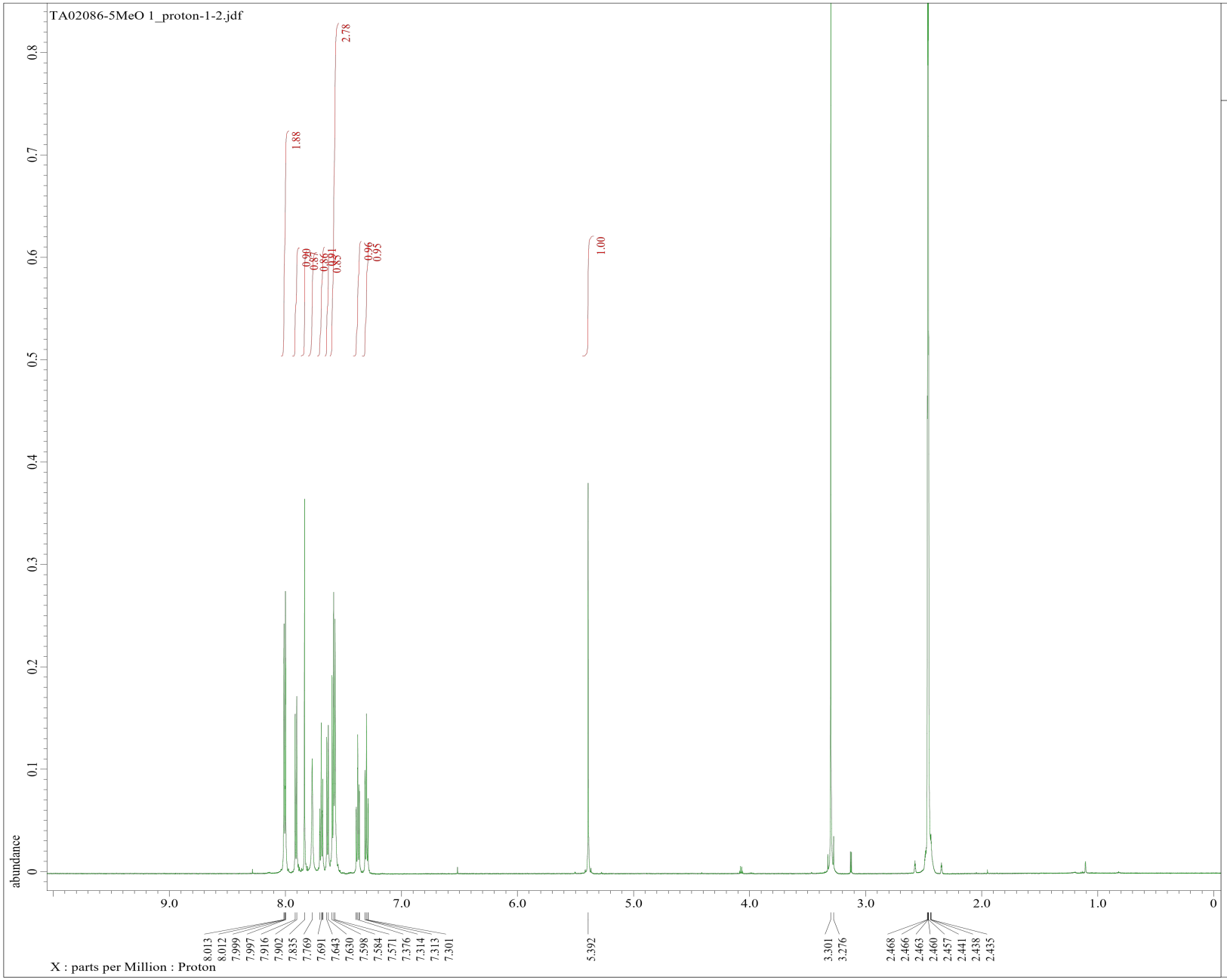
Filename	= TA201121-1_proton-1-3
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA201121-1
Solvent	= DMSO-D6
Actual_Start_Time	= 21-NOV-2020 08:45:06
Revision_Time	= 21-NOV-2020 09:01:38
Comment	= 7F-HITAB
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 2.9097984[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.34366642[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 46
Temp_Get	= 20.4[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 2.9097984[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	= 3.9097984[s]



3ha

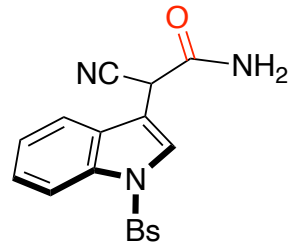

TA201121-2_carbon-1-2.jdf
(thousandths)
X : parts per Million : Carbon13
165.357
150.143
148.487
146.457
134.766
132.602
130.898
129.280
127.920
125.517
125.469
121.830
121.754
117.407
116.660
112.600
112.438
112.304
40.550
40.426
40.292
40.158
40.014
39.870
39.736
39.593
36.309
21.650


Filename = TA201121-2_carbon-
Author = delta
Experiment = carbon.jxp
Sample_Id = TA201121-2
Solvent = DMSO-D6
Actual_Start_Time = 21-NOV-2020 08:57:
Revision_Time = 21-NOV-2020 11:42:
Comment = single pulse decou
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 = 5000
Total_Scans = 5000
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 19.3[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]
O
NC
NH2
N
F
Ts
3ha

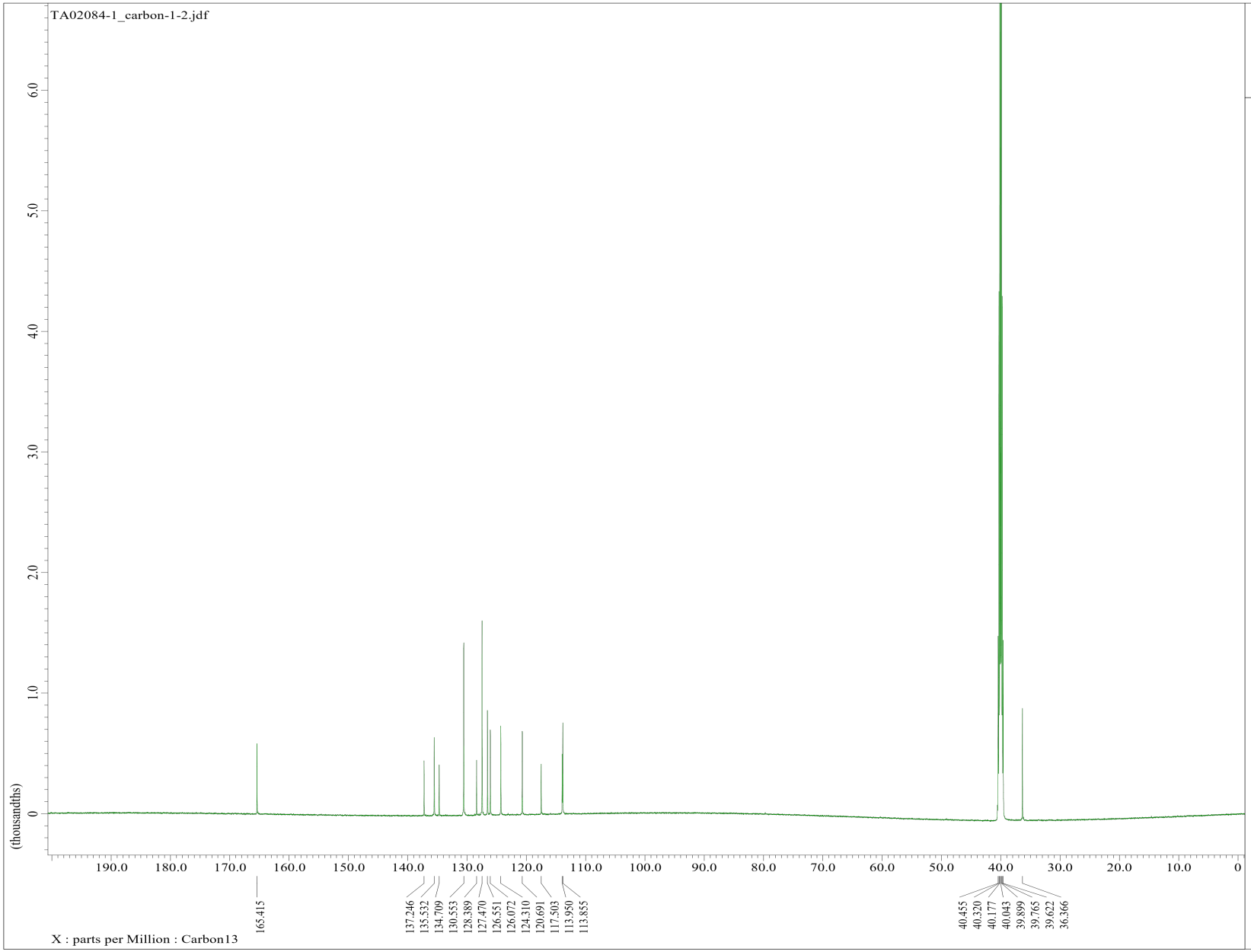


JEOL

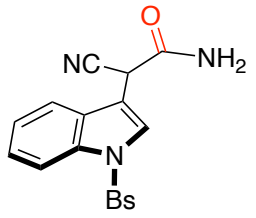
Filename	= TA02086-5MeO 1_proton
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA02086-5MeO 1
Solvent	= DMSO-D6
Actual_Start_Time	= 11-NOV-2020 08:48:20
Revision_Time	= 11-NOV-2020 08:50:12
Comment	= single_pulse-5MeO
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
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	= 5[us]
Clipped	= TRUE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 19.5[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 2.90455552[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	= 3.90455552[s]



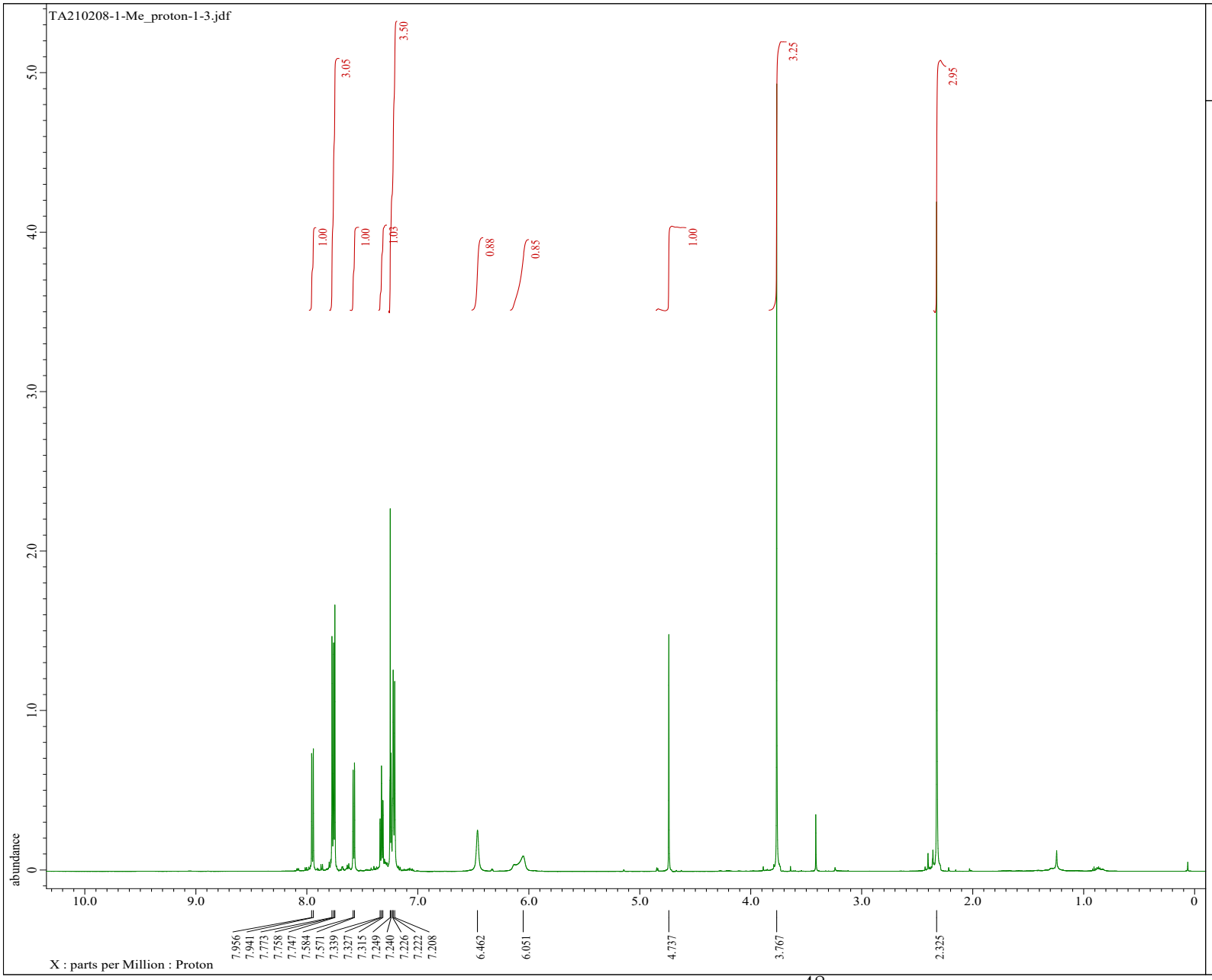
3ia



Filename	= TA02084-1_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA02084-1
Solvent	= DMSO-D6
Actual_Start_Time	= 11-NOV-2020 00:02:
Revision_Time	= 11-NOV-2020 20:38:
Comment	= single pulse decou
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	= 6000
Total_Scans	= 6000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 36
Temp_Get	= 19.5[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]

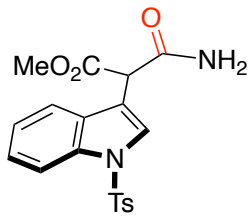


3ia

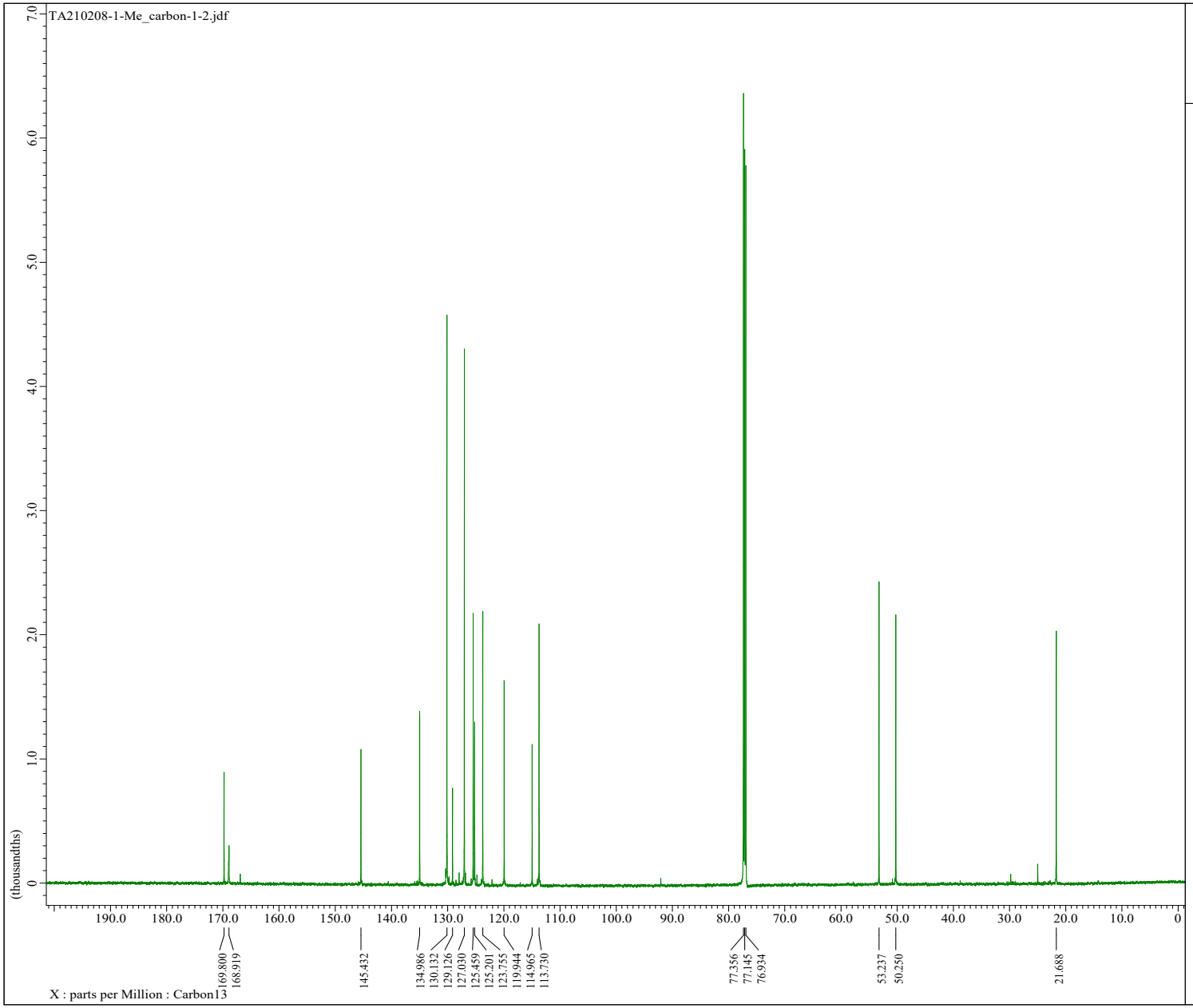


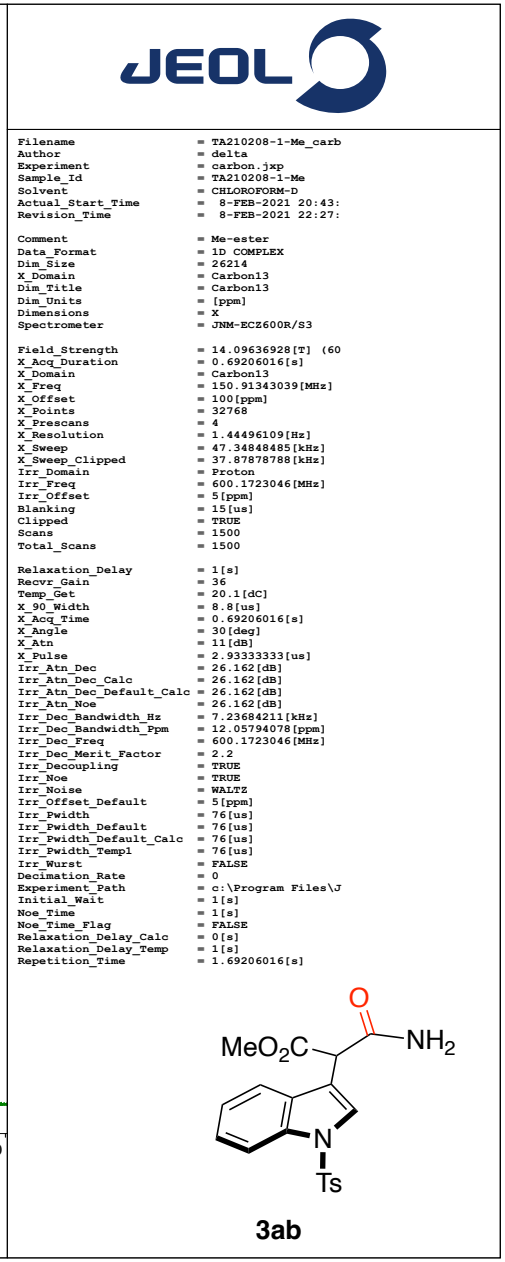
JEOL

Filename	= TA210208-1-Me_proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210208-1-Me
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-FEB-2021 20:39:38
Revision_Time	= 8-FEB-2021 20:44:36
Comment	= Me-ester
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.09051904[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.91699454[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	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.2[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.09051904[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.09051904[s]

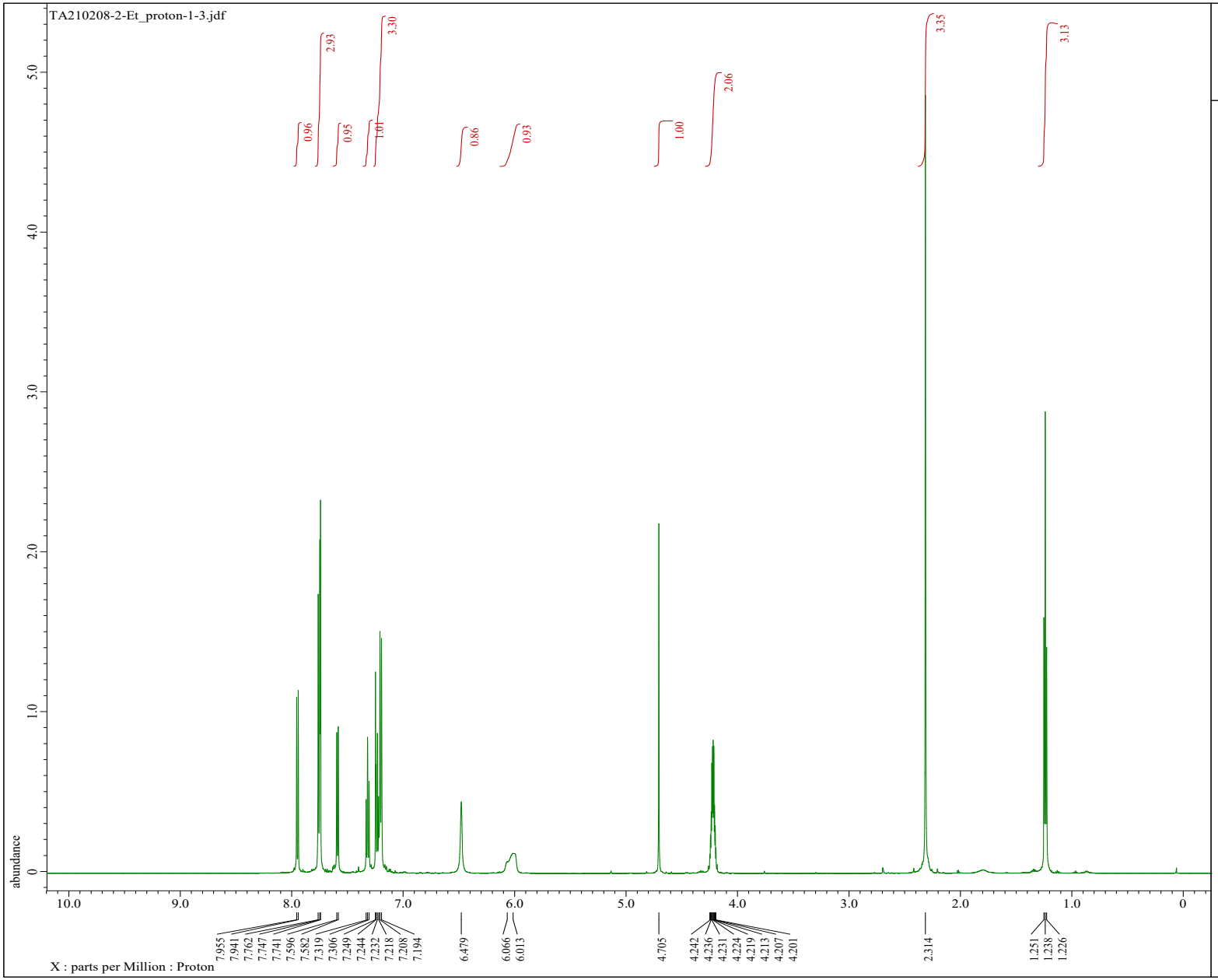


3ab

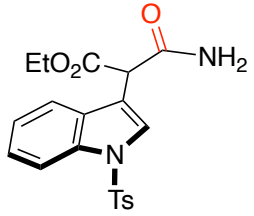

TA210208-1-Me_carbon-1-2.jdf
(thousandths)
X : parts per Million : Carbon13
169.800
168.919
145.432
134.986
130.132
129.126
127.030
125.459
125.201
123.755
119.944
114.965
113.730
77.356
77.145
76.934
53.237
50.250
21.688


Filename = TA210208-1-Me_carb
Author = delta
Experiment = carbon.jxp
Sample_Id = TA210208-1-Me
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-FEB-2021 20:43:
Revision_Time = 8-FEB-2021 22:27:
Comment = Me-ester
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 = 150.9134039[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 = 1500
Total_Scans = 1500
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_Templ = 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]
O
MeO2C
NH2
N
Ts

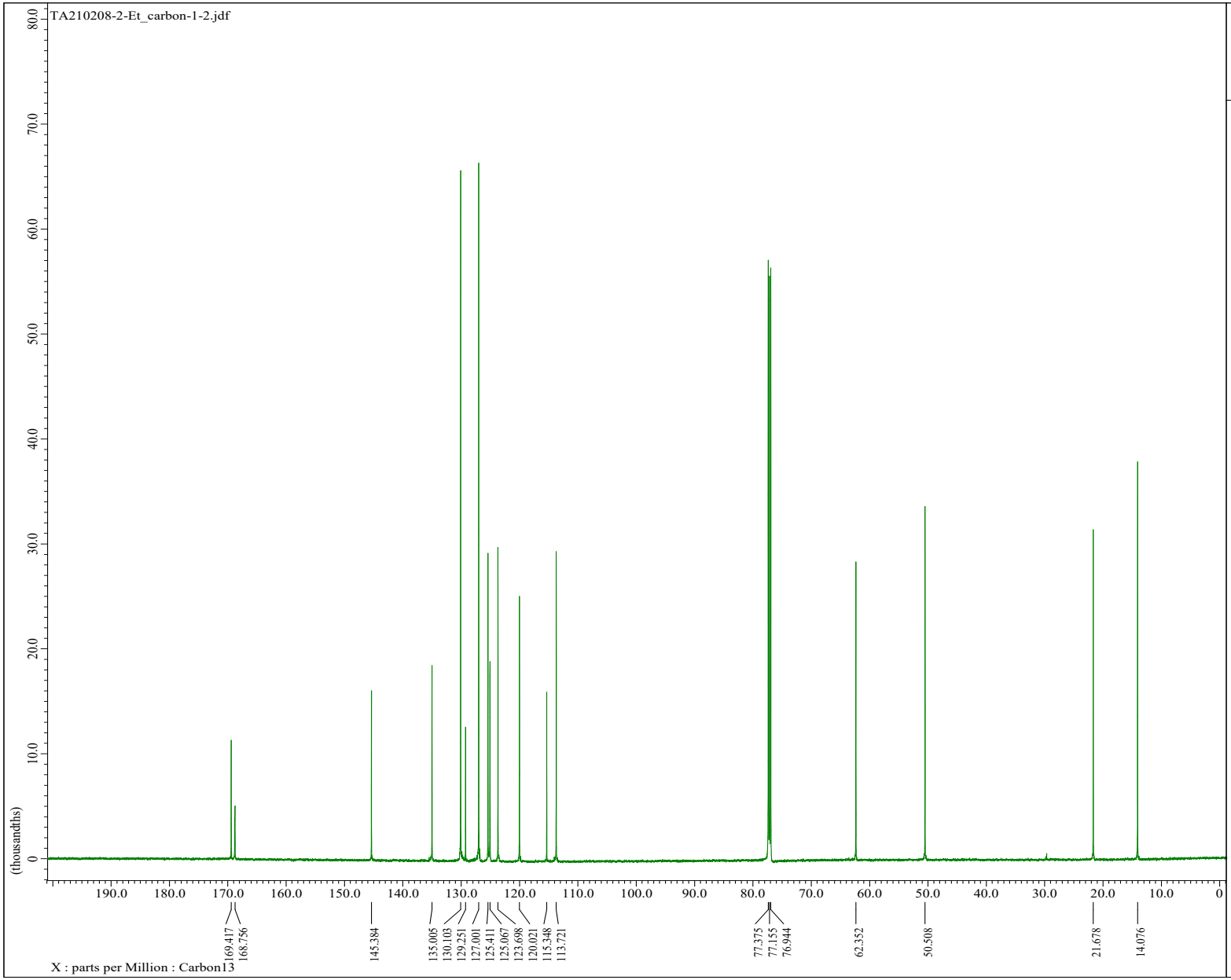
3ab



Filename	= TA210208-2-Et_proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210208-2-Et
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-FEB-2021 21:39:14
Revision_Time	= 8-FEB-2021 22:38:27
Comment	= Et-ester
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.09051904[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.91699454[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	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.09051904[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.09051904[s]

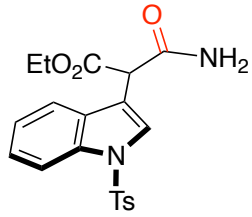


3ac

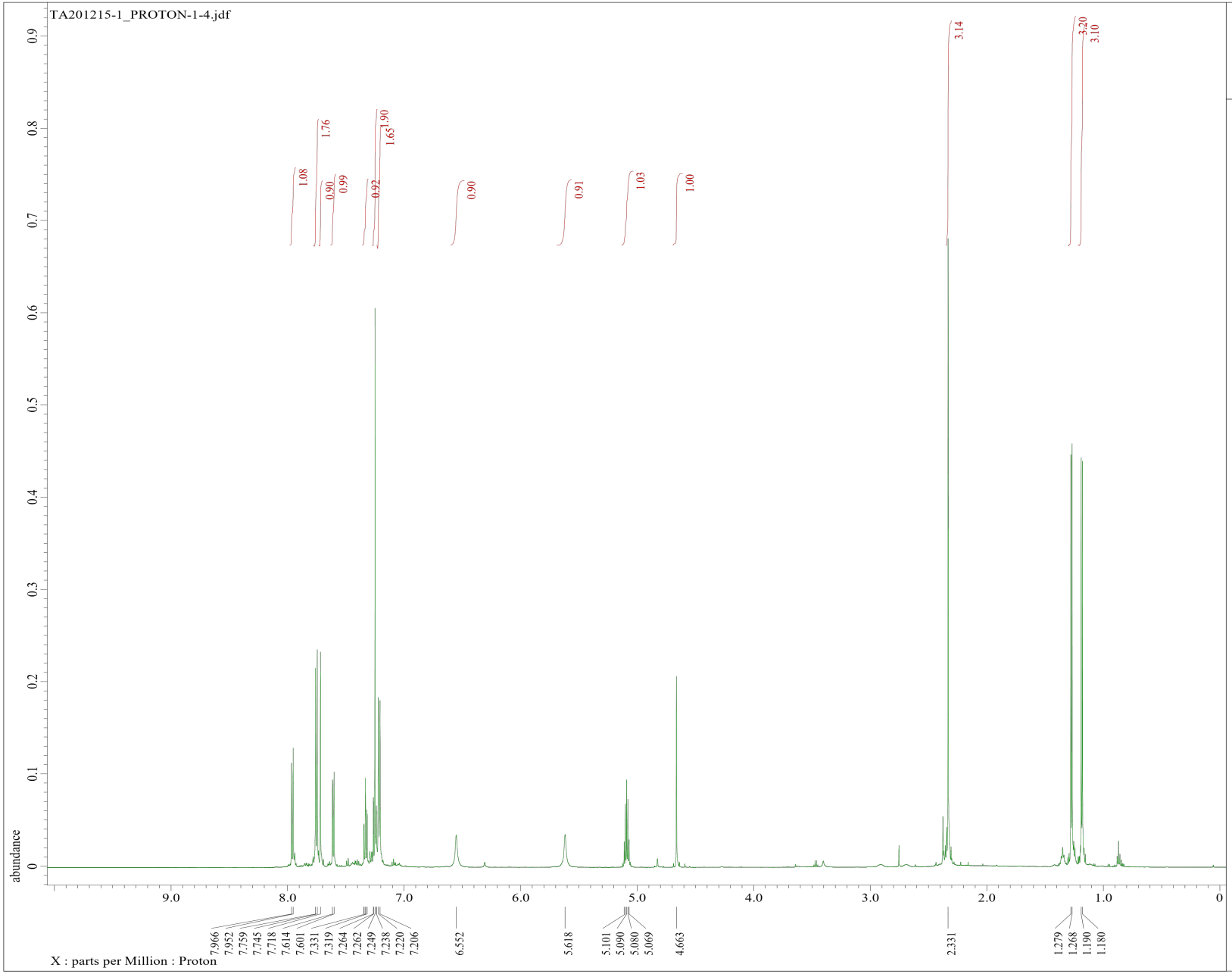


JEOL

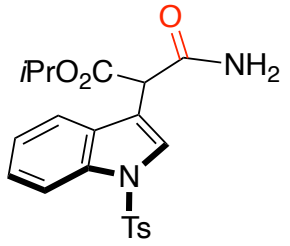
Filename	= TA210208-2-Et_carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210208-2-Et
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-FEB-2021 21:43:
Revision_Time	= 8-FEB-2021 22:30:
Comment	= Et-ester
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [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	= 1500
Total_Scans	= 1500
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
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]



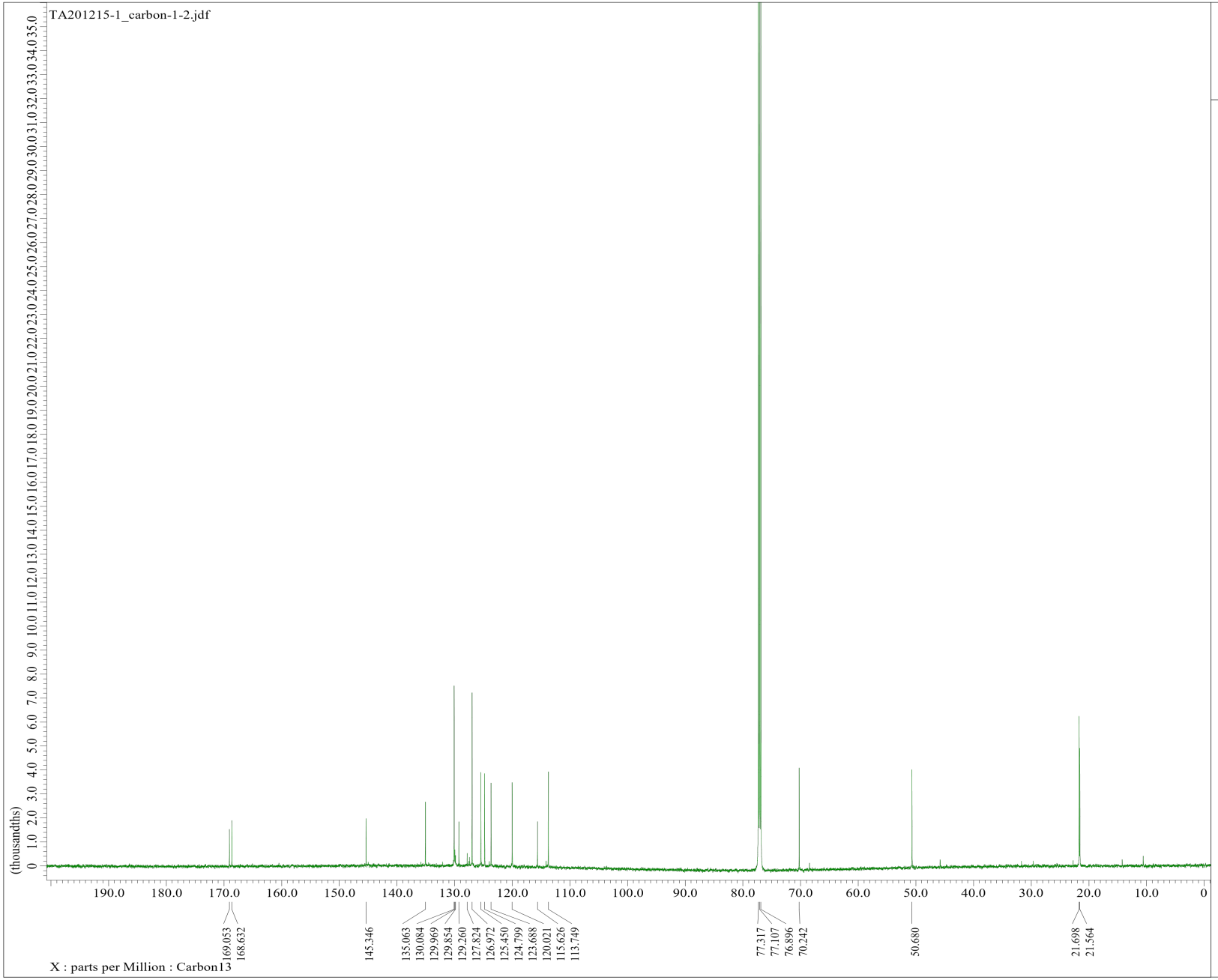
3ac




```
Filename                = TA201215-1_PROTON-1-4
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TA201215-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 15-DEC-2020 20:33:04
Revision_Time           = 15-DEC-2020 20:37:51

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

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 2.90455552[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 32768
X_Prescans              = 0
X_Resolution            = 0.34428676[Hz]
X_Sweep                 = 11.28158845[kHz]
X_Sweep_Clipped         = 9.02527076[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 4[s]
Recvr_Gain              = 42
Temp_Get                = 20.7[dC]
X_90_Width              = 9.5[us]
X_Acq_Time              = 2.90455552[s]
X_Angle                 = 45[deg]
X_Atn                   = 8.1[dB]
X_Pulse                 = 4.75[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 400
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = c:\Program Files\JEOL
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 4[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 4[s]
Repetition_Time         = 6.90455552[s]
```

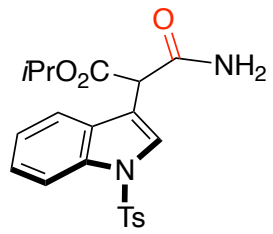


3ad

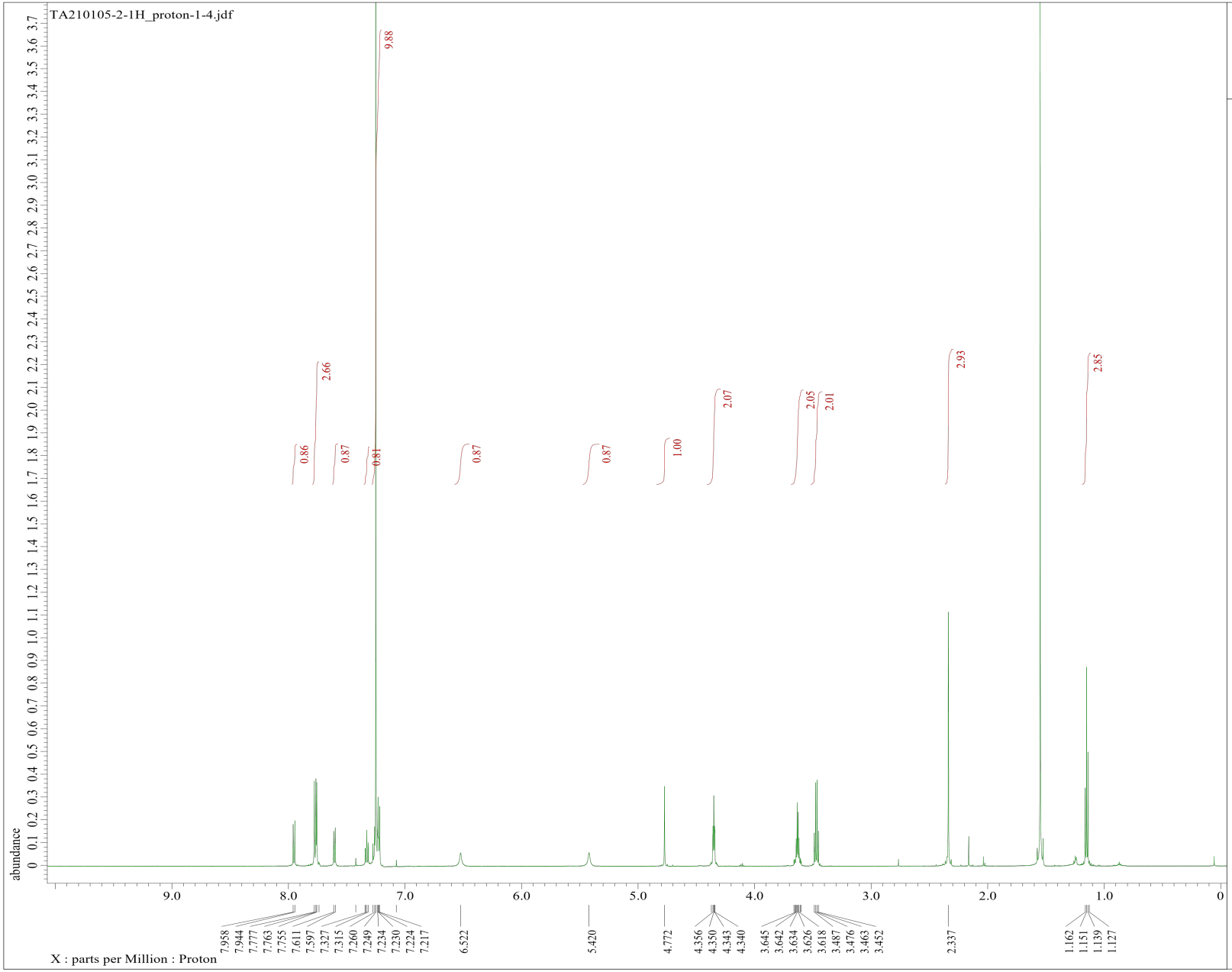


JEOL

Filename	= TA201215-1_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA201215-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-DEC-2020 20:37:
Revision_Time	= 15-DEC-2020 22:25:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-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	= 3000
Total_Scans	= 3000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[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]

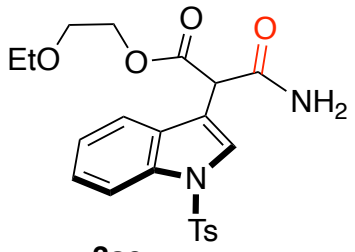


3ad

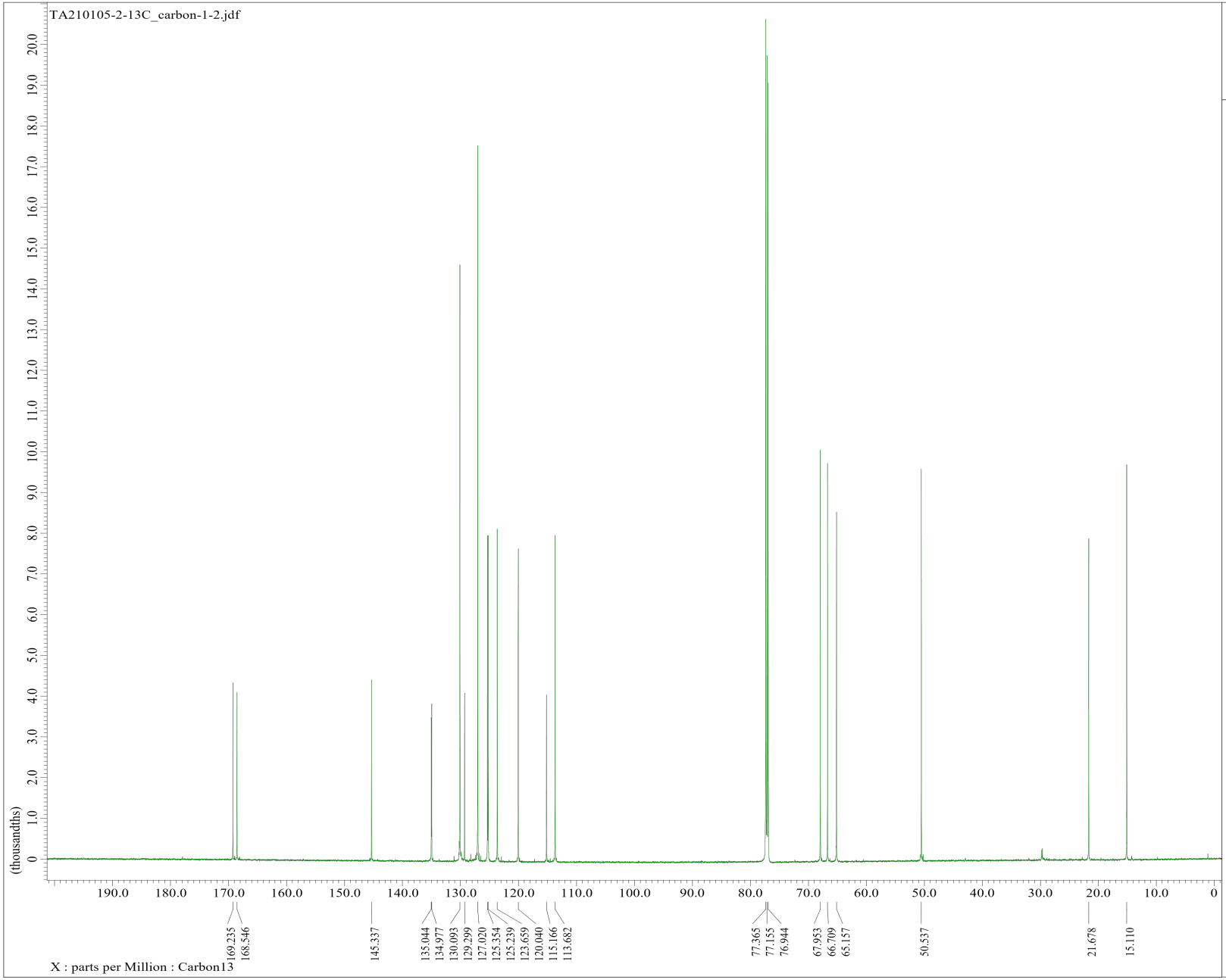


JEOL

```
Filename              = TA210105-2-1H_proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TA210105-2-1H
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  5-JAN-2021 21:14:52
Revision_Time         =  5-JAN-2021 21:23:34

Comment               = single_pulse-EtOCH2CH
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
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        = 1.4548992[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.68733284[Hz]
X_Sweep               = 11.26126126[kHz]
X_Sweep_Clipped       = 9.00900901[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      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 20.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 1.4548992[s]
X_Angle               = 45[deg]
X_Atn                 = 8.1[dB]
X_Pulse               = 4.75[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       = 6.4548992[s]
```

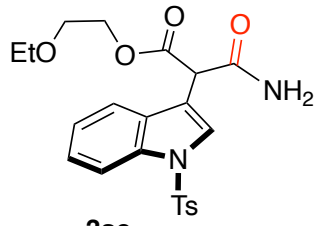


3ae

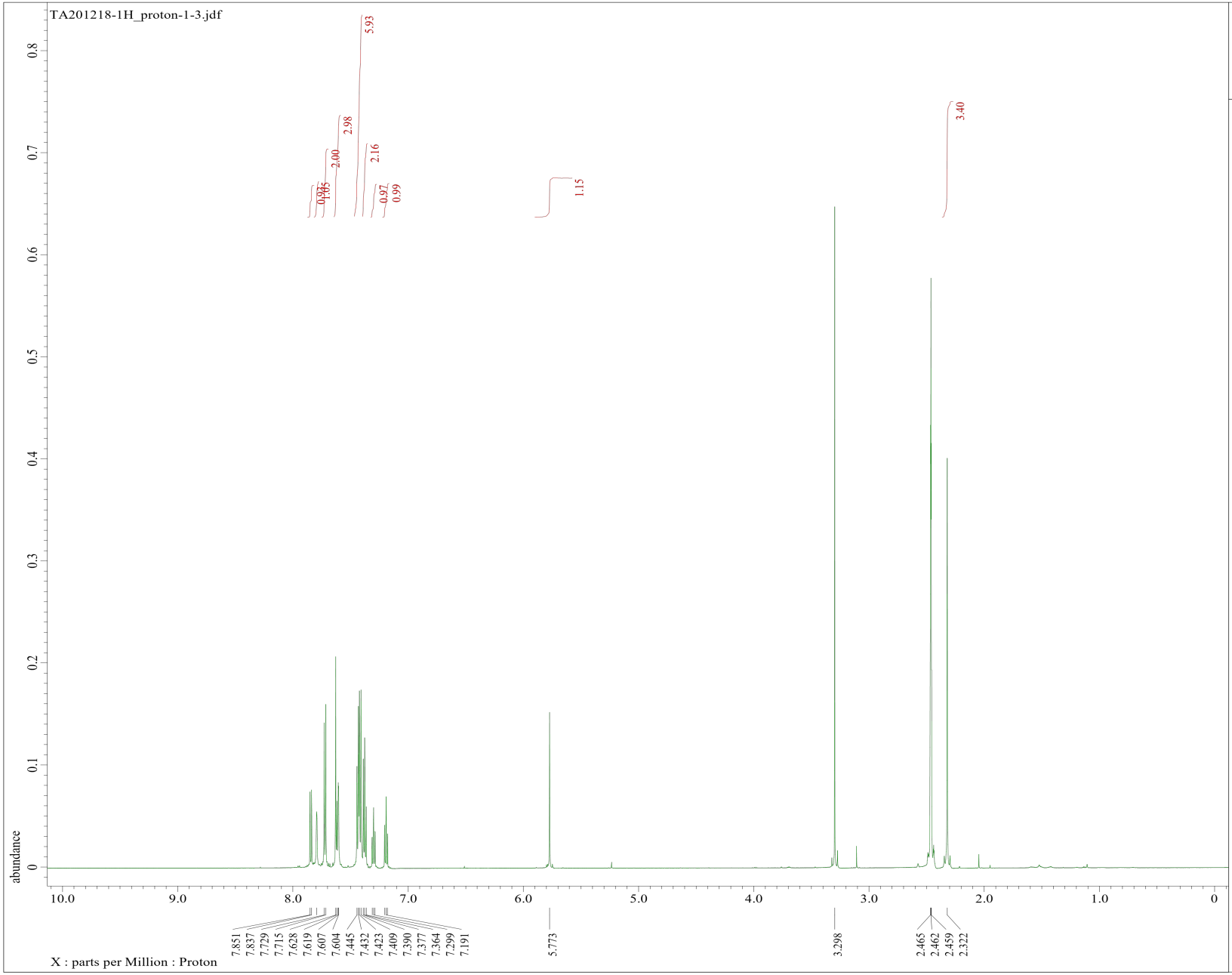


JEOL

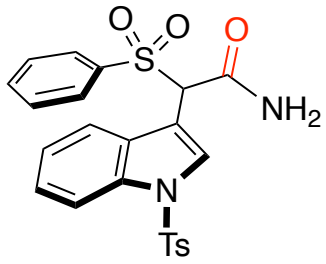
Filename	= TA210105-2-13C_car
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210105-2-13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JAN-2021 21:31:
Revision_Time	= 6-JAN-2021 08:10:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
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	= 7000
Total_Scans	= 7000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 46
Temp_Get	= 19.7[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]



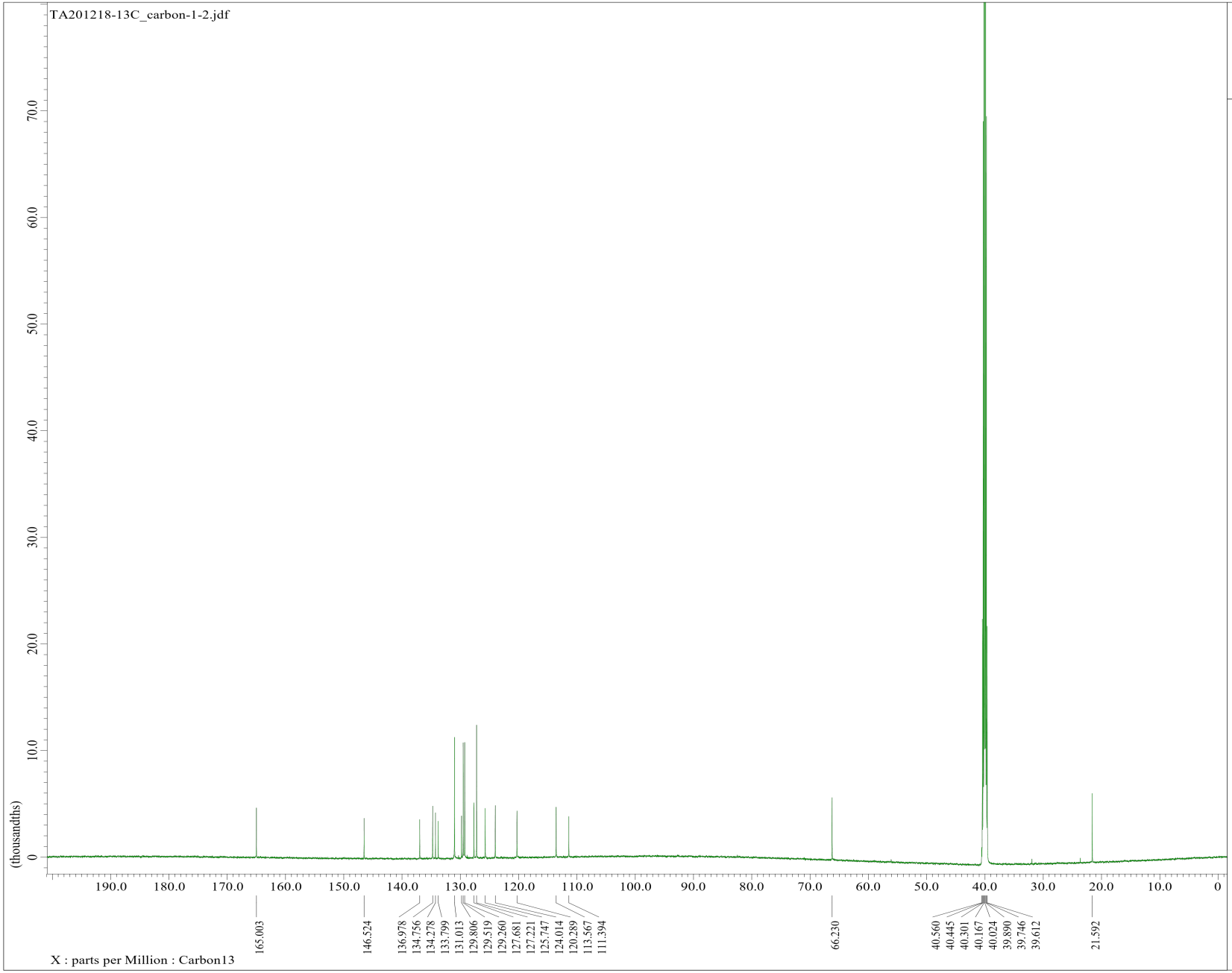
3ae




```
Filename                = TA201218-1H_proton-1-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TA201218-1H
Solvent                 = DMSO-D6
Actual_Start_Time       = 18-DEC-2020 14:06:33
Revision_Time           = 18-DEC-2020 14:18:20

Comment                 = single_pulse-PhSO2-
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
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          = 1.09051904[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.91699454[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        = 5[s]
Recvr_Gain              = 36
Temp_Get                = 20.4[dC]
X_90_Width              = 9.5[us]
X_Acq_Time              = 1.09051904[s]
X_Angle                 = 45[deg]
X_Atn                   = 8.1[dB]
X_Pulse                 = 4.75[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         = 6.09051904[s]
```

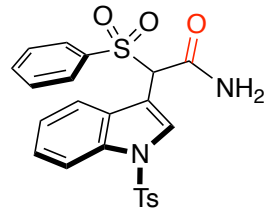


3af

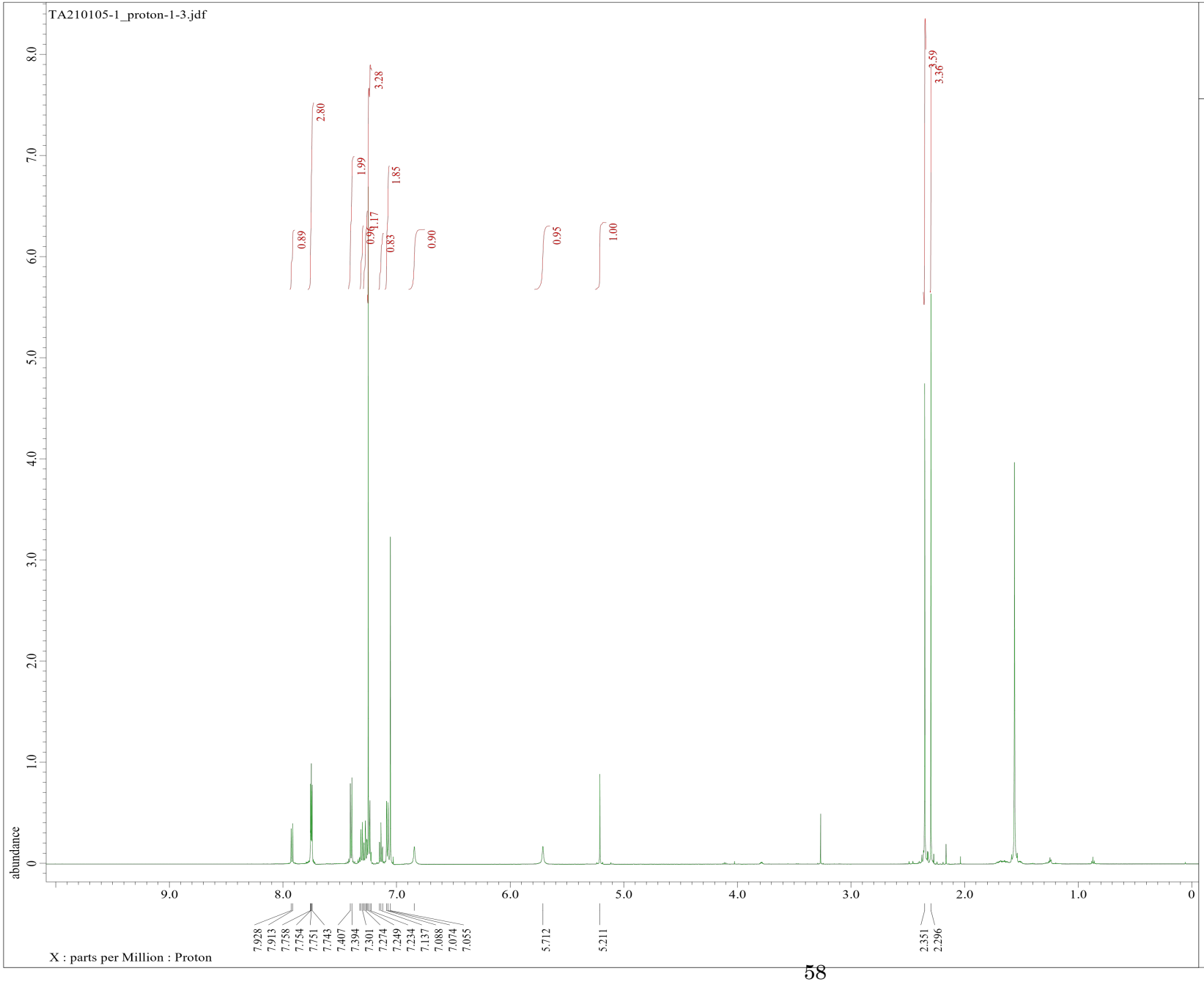


JEOL

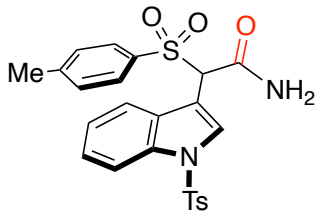
Filename	= TA201218-13C_carbo
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA201218-13C
Solvent	= DMSO-D6
Actual_Start_Time	= 18-DEC-2020 14:14:
Revision_Time	= 18-DEC-2020 15:14:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [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	= 1800
Total_Scans	= 1800
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.5[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]



3af




```
Filename                = TA210105-1_proton-1-3
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TA210105-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  5-JAN-2021 21:08:10
Revision_Time           =  5-JAN-2021 21:26:27

Comment                 = single_pulse-a-Ts-ind
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
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          = 1.4548992[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.68733284[Hz]
X_Sweep                 = 11.26126126[kHz]
X_Sweep_Clipped         = 9.00900901[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        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 20.1[dC]
X_90_Width              = 9.5[us]
X_Acq_Time              = 1.4548992[s]
X_Angle                 = 45[deg]
X_Atn                   = 8.1[dB]
X_Pulse                 = 4.75[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         = 6.4548992[s]
```



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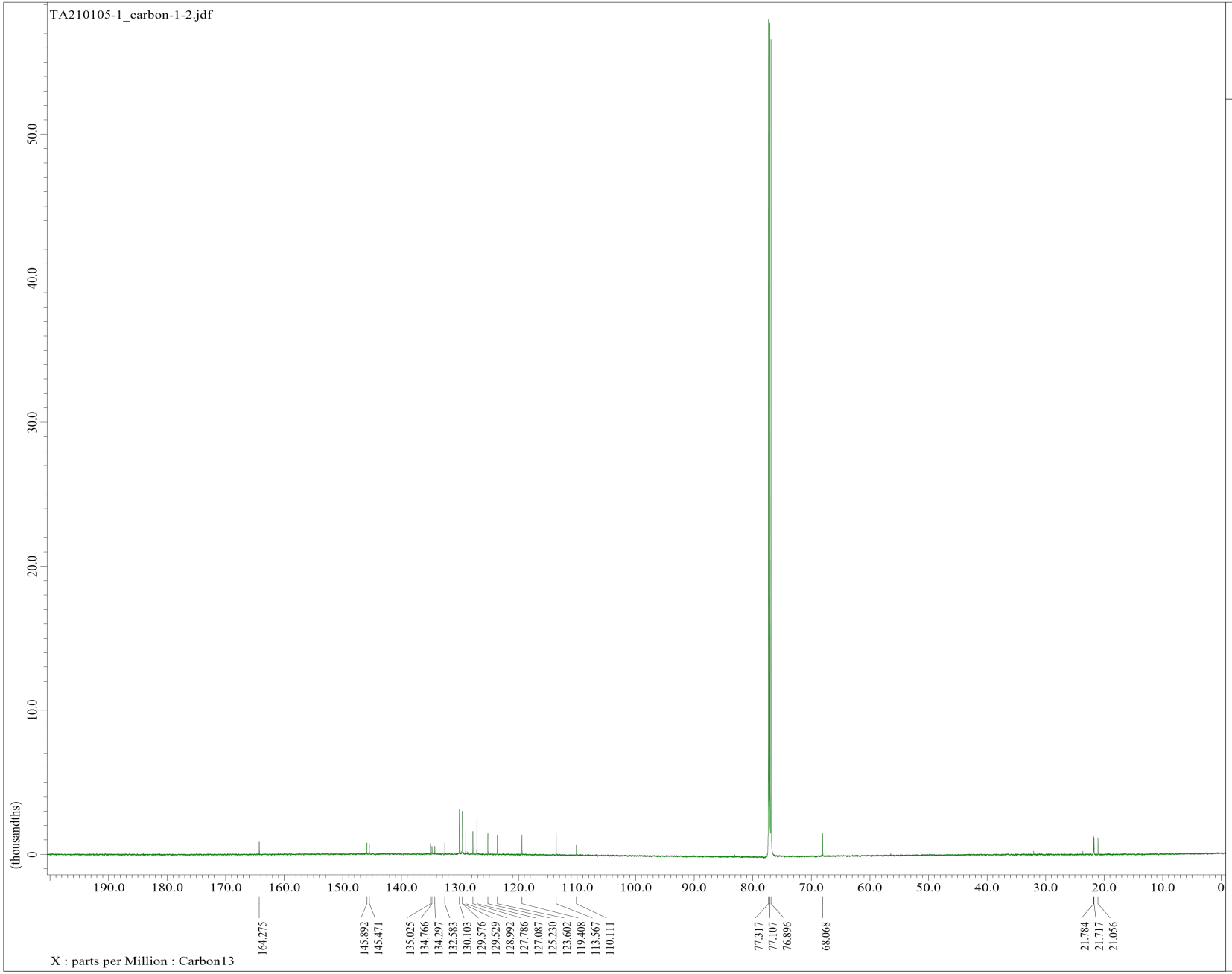
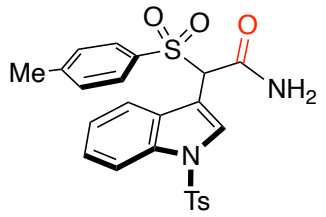


```
Filename                = TA210105-1_carbon-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = TA210105-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  6-JAN-2021 01:32:
Revision_Time           =  6-JAN-2021 08:11:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-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                   = 7000
Total_Scans             = 7000

Relaxation_Delay        = 1[s]
Recvr_Gain              = 56
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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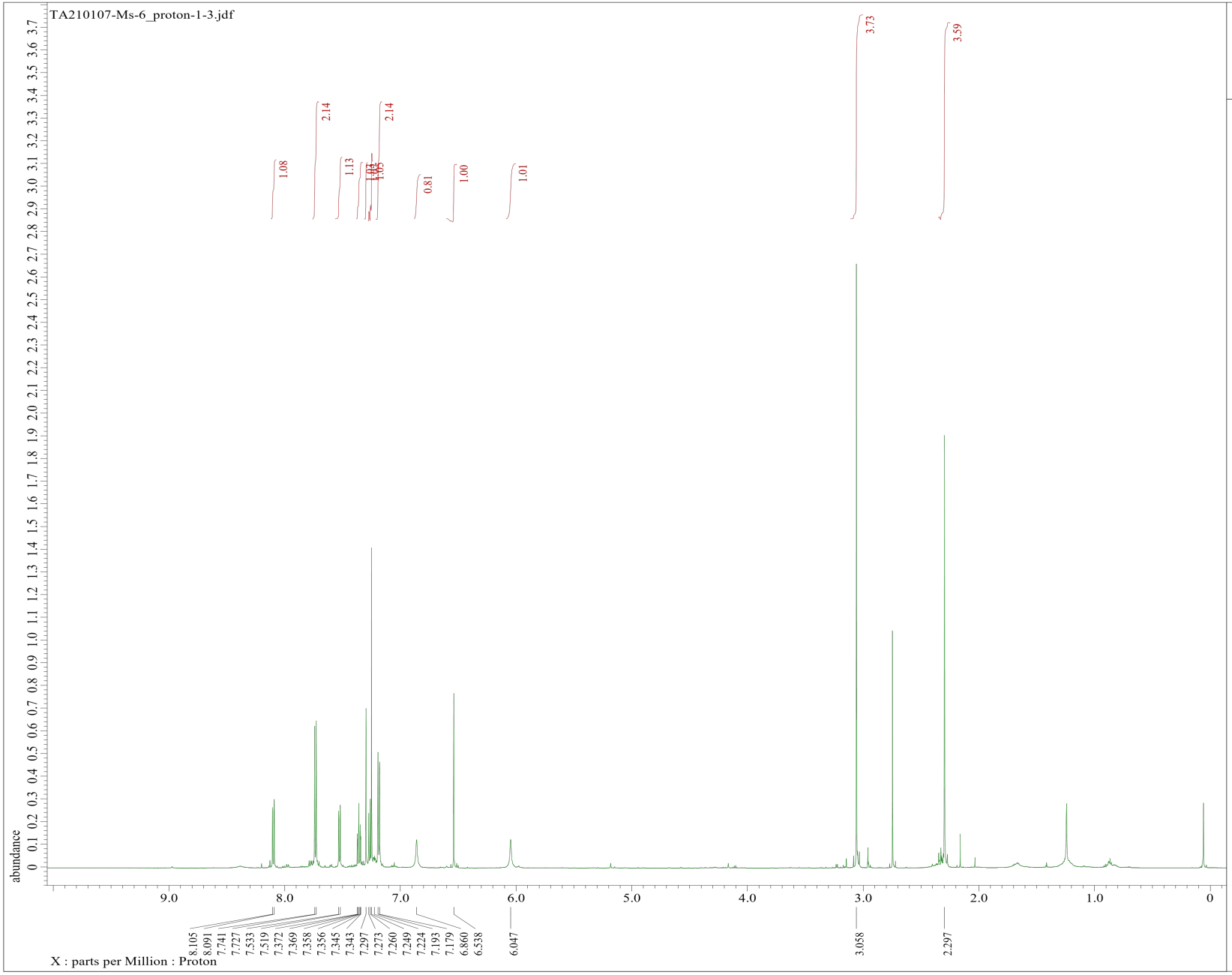
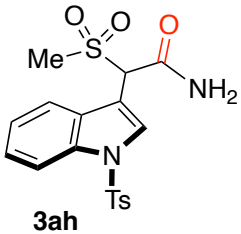


JEOL

Filename	= TA210107-Ms-6_proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210107-Ms-6
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-JAN-2021 21:21:42
Revision_Time	= 7-JAN-2021 21:28:44
Comment	= single_pulse-MsCH2CN-
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.2[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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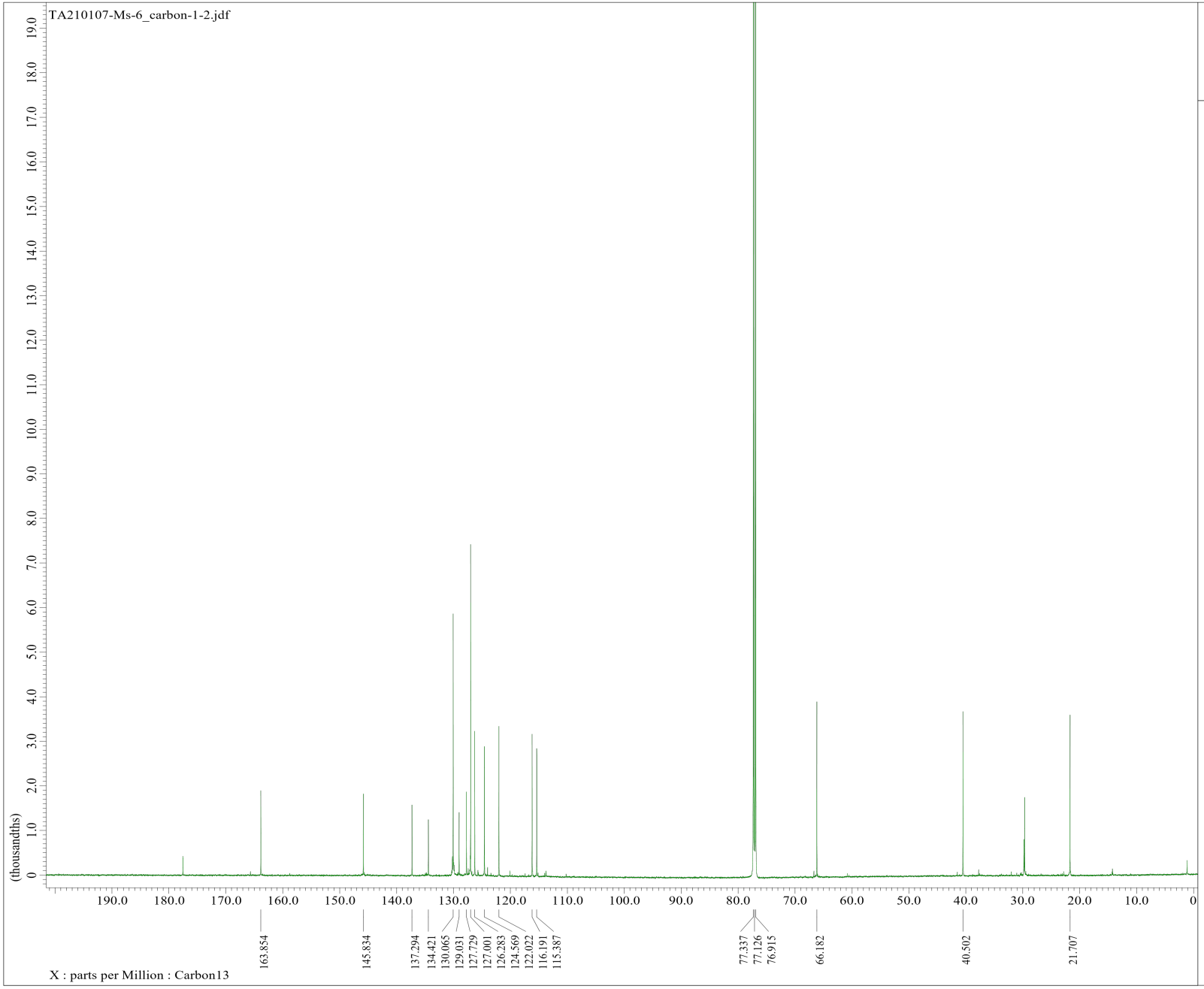
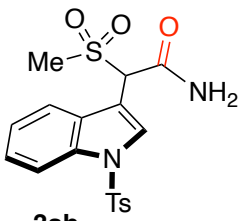


JEOL

Filename	= TA210107-Ms-6_carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210107-Ms-6
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-JAN-2021 21:26:
Revision_Time	= 8-JAN-2021 08:24:
Comment	= single pulse decou
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	= 8000
Total_Scans	= 8000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 46
Temp_Get	= 20.2[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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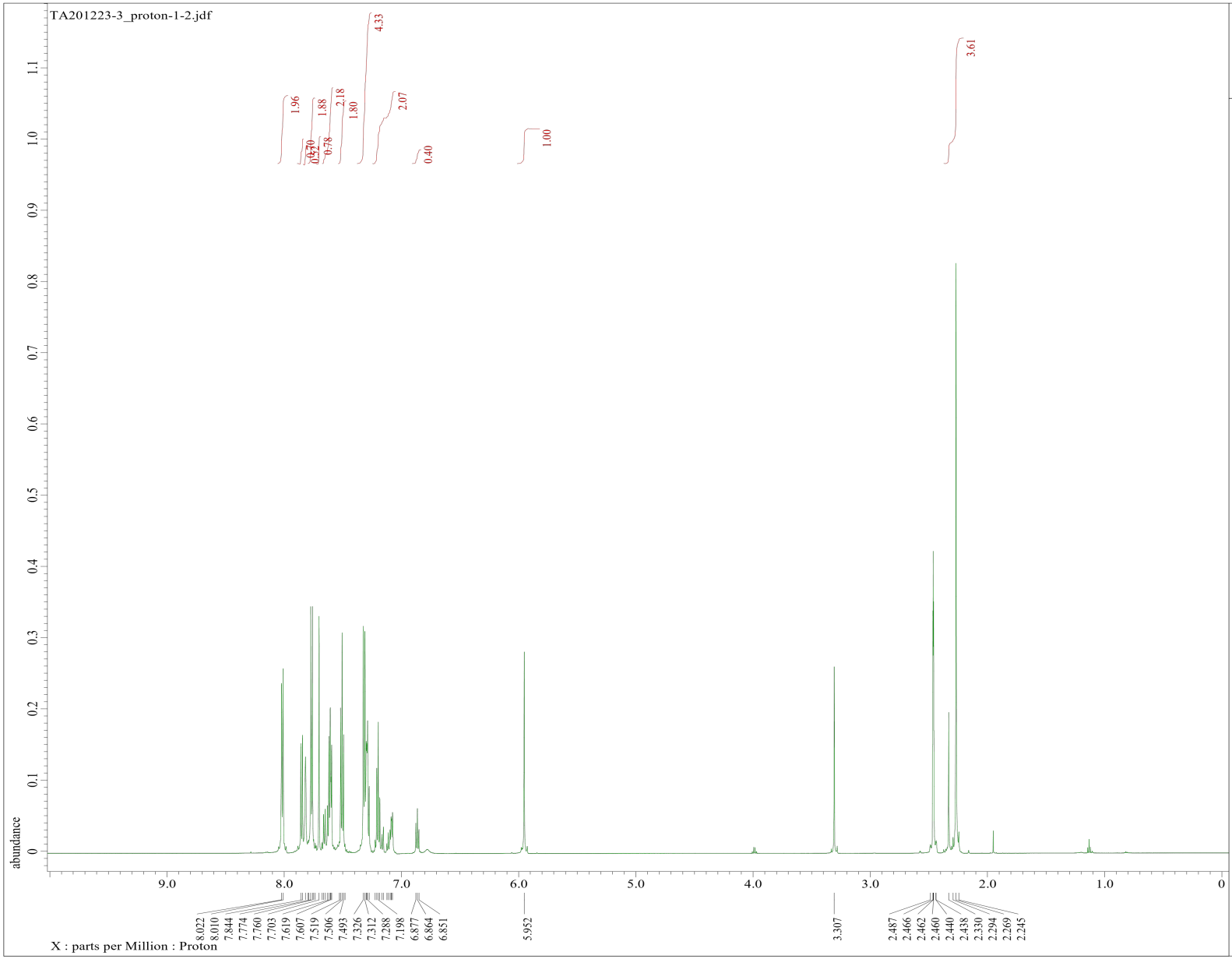
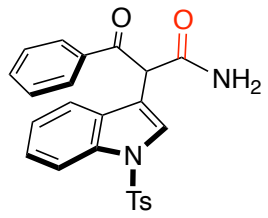


Filename	= TA201223-3_proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA201223-3
Solvent	= DMSO-D6
Actual_Start_Time	= 23-DEC-2020 22:14:21
Revision_Time	= 23-DEC-2020 22:18:59
Comment	= single_pulse-Bz-indol
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 19.6[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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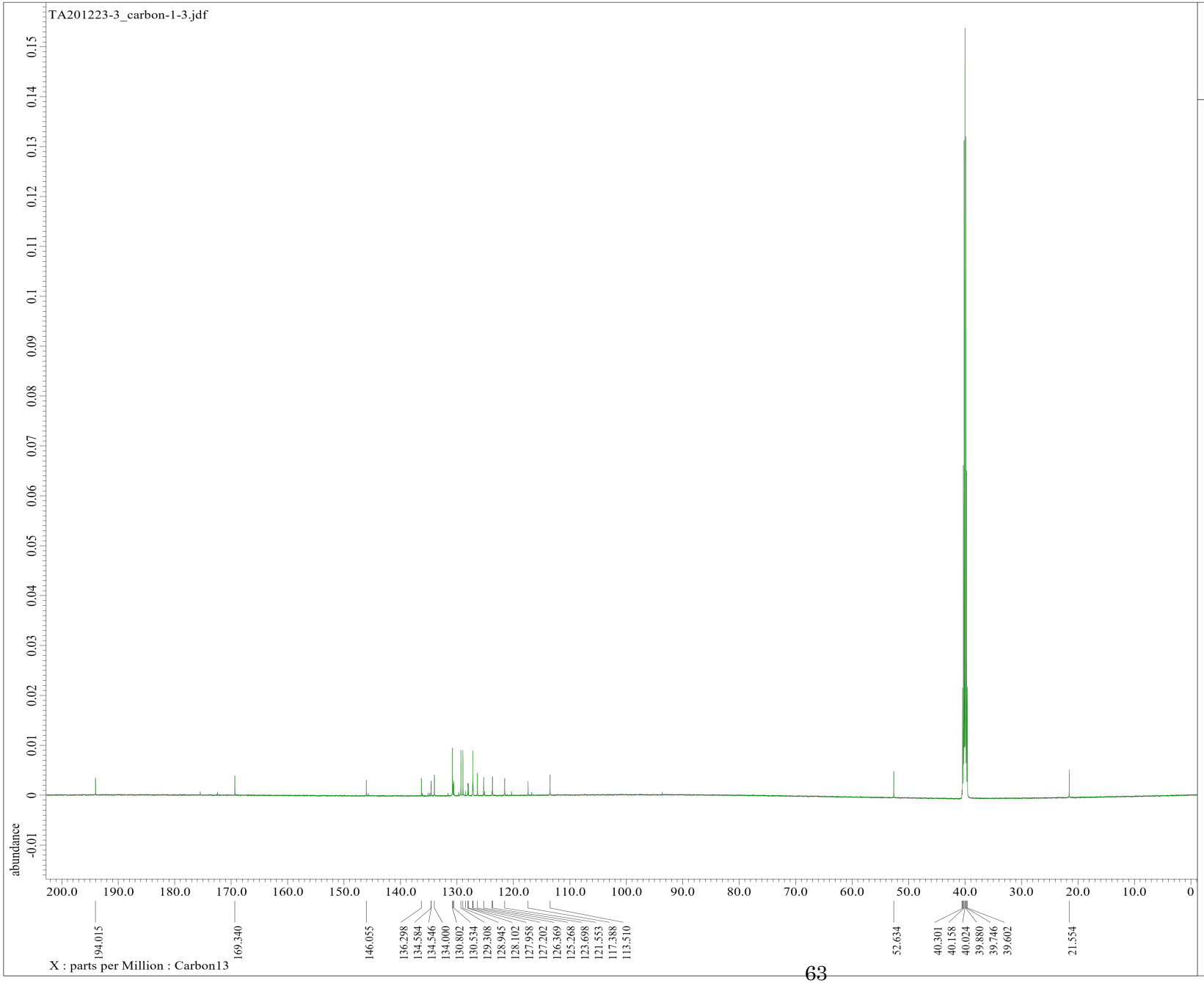
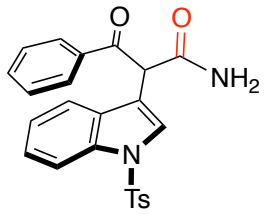


JEOL

Filename	= TA201223-3_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA201223-3
Solvent	= DMSO-D6
Actual_Start_Time	= 23-DEC-2020 22:19:
Revision_Time	= 24-DEC-2020 08:10:
Comment	= single pulse decou
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	= 1300
Total_Scans	= 1300
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 19.8[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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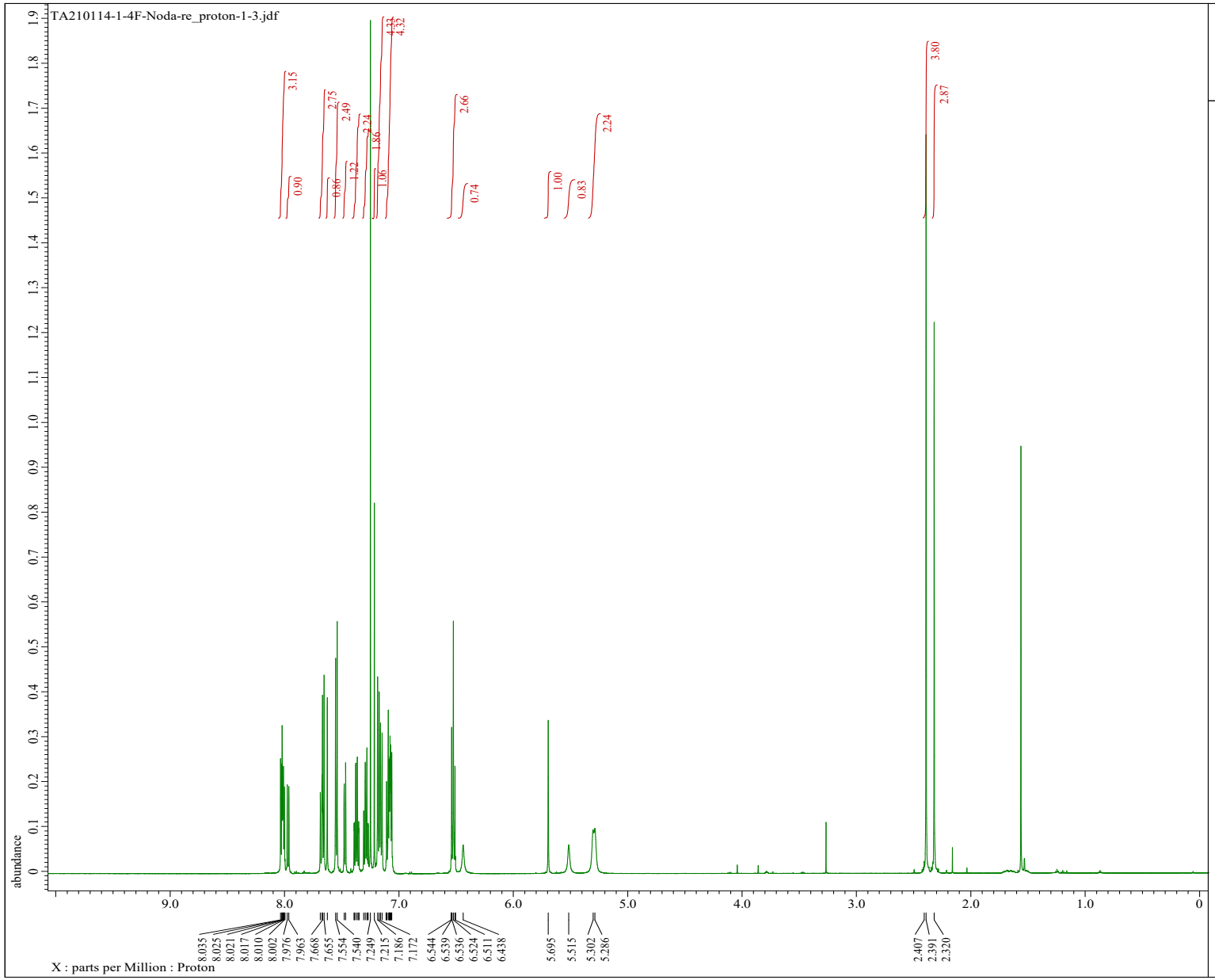
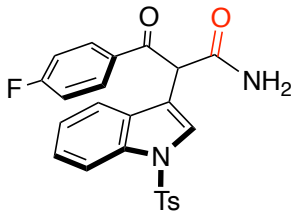


JEOL

Filename	= TA210114-1-4F-Noda-re
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210114-1-4F-Noda-re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-JAN-2021 20:46:26
Revision_Time	= 17-JAN-2021 18:36:12
Comment	= 4F-indolylacetamide
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 20.4[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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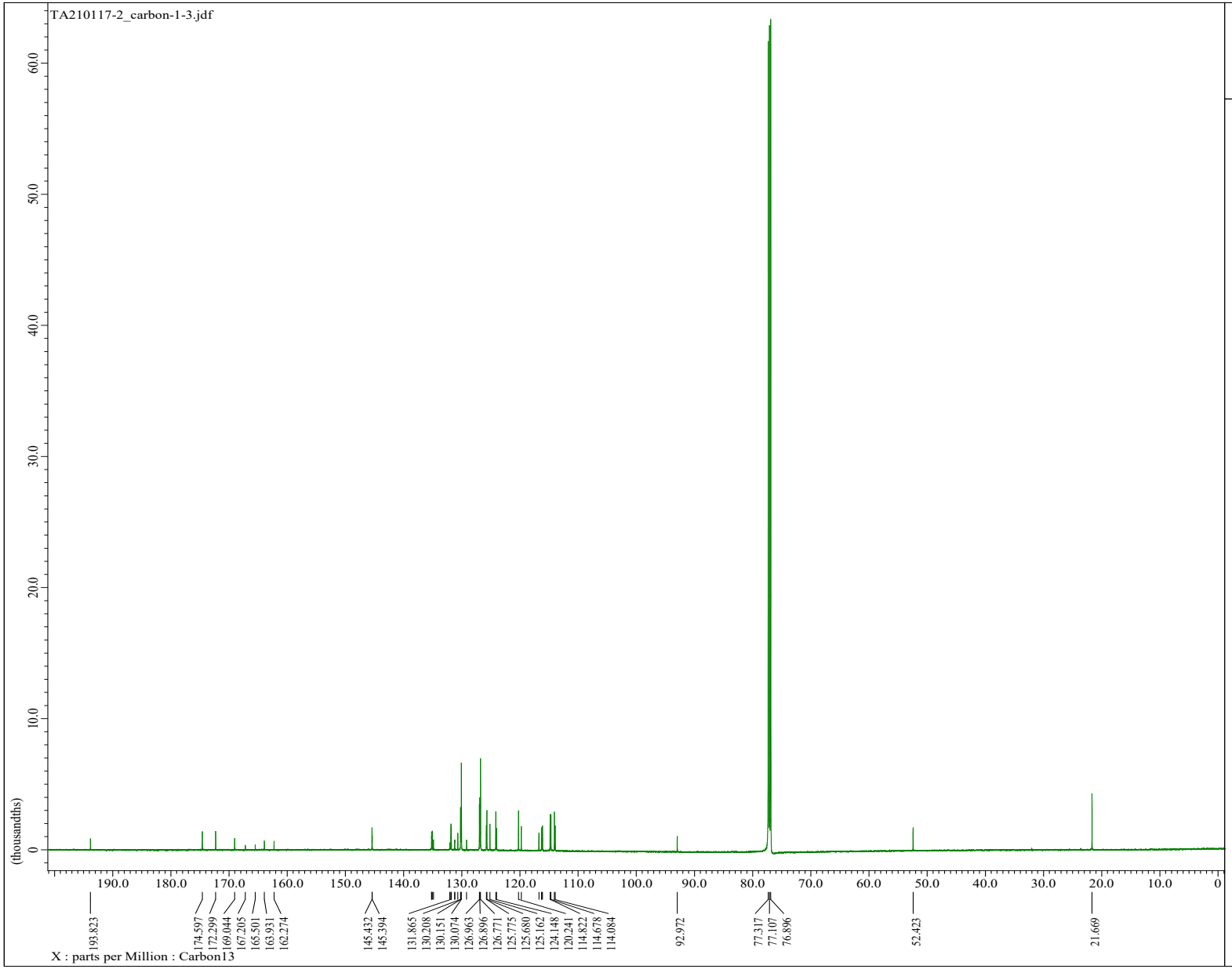
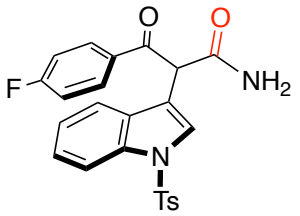


Filename	= TA210117-2_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210117-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-JAN-2021 22:03:
Revision_Time	= 18-JAN-2021 08:01:
Comment	= 4F-enol
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [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	= 10000
Total_Scans	= 10000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.5[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_Templ	= 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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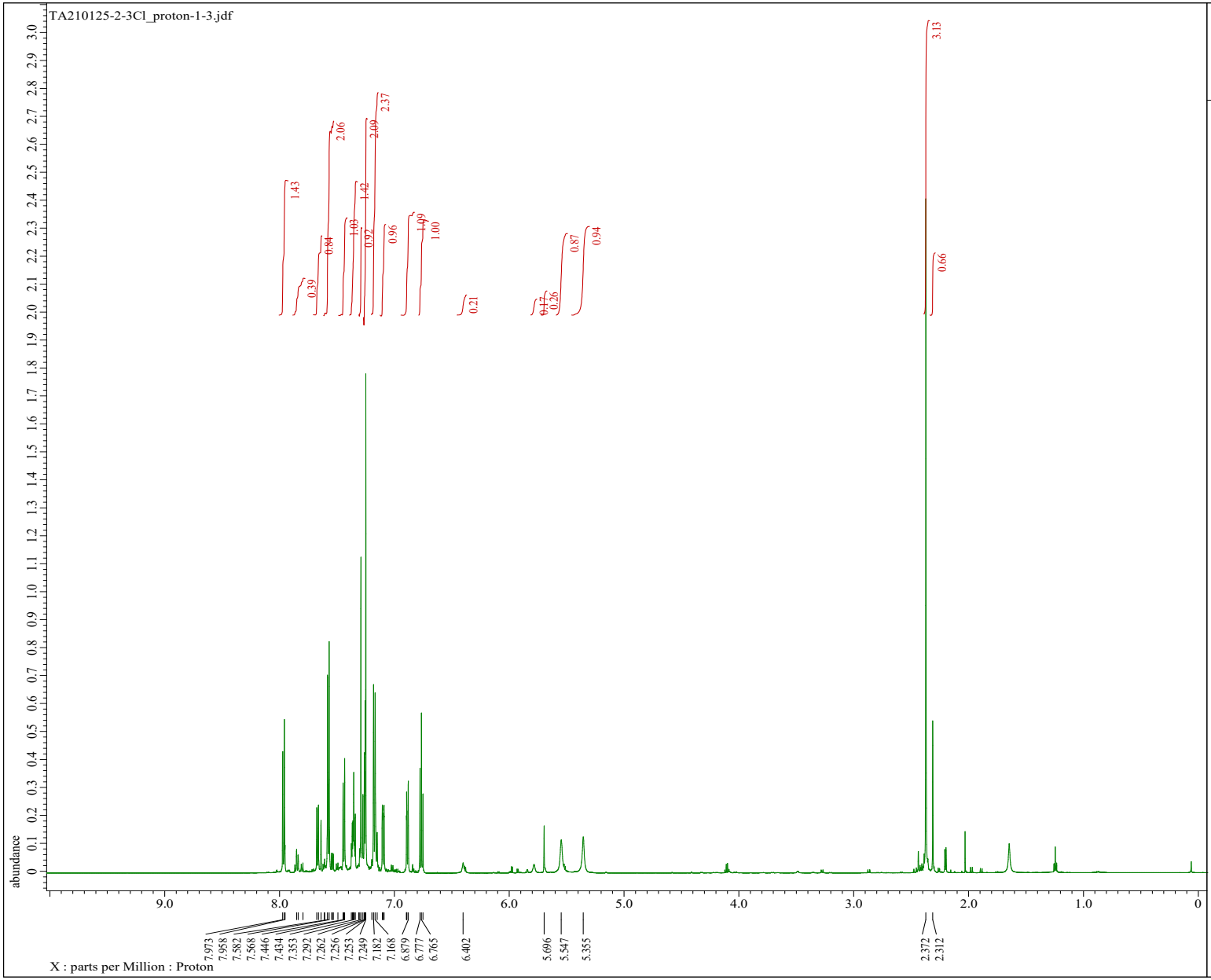
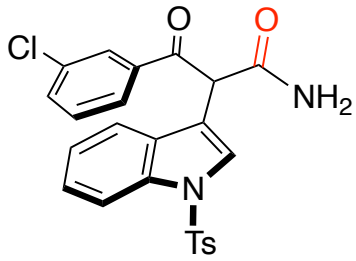


JEOL

Filename	= TA210125-2-3Cl_proton
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210125-2-3Cl
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JAN-2021 20:31:11
Revision_Time	= 28-JAN-2021 13:33:30
Comment	= 3Cl-benzoylacetonitri
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.6[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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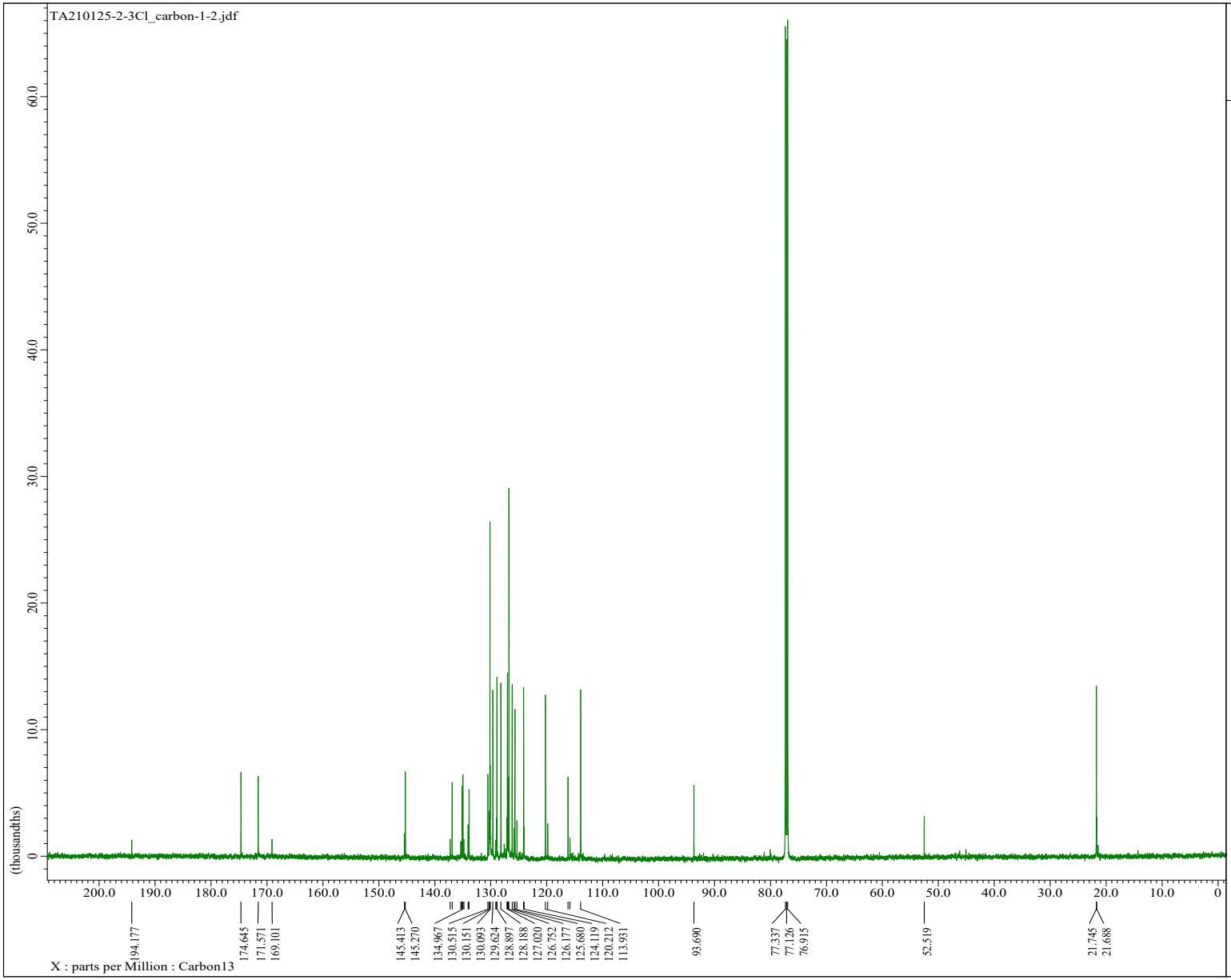
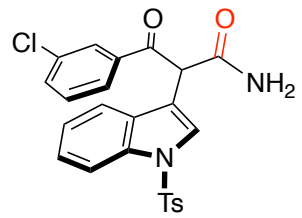


JEOL

Filename	= TA210125-2-3Cl_car
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210125-2-3Cl
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JAN-2021 20:35:
Revision_Time	= 25-JAN-2021 21:30:
Comment	= 3-Cl-benzoylaceton
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	= 350
Total_Scans	= 350
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.7[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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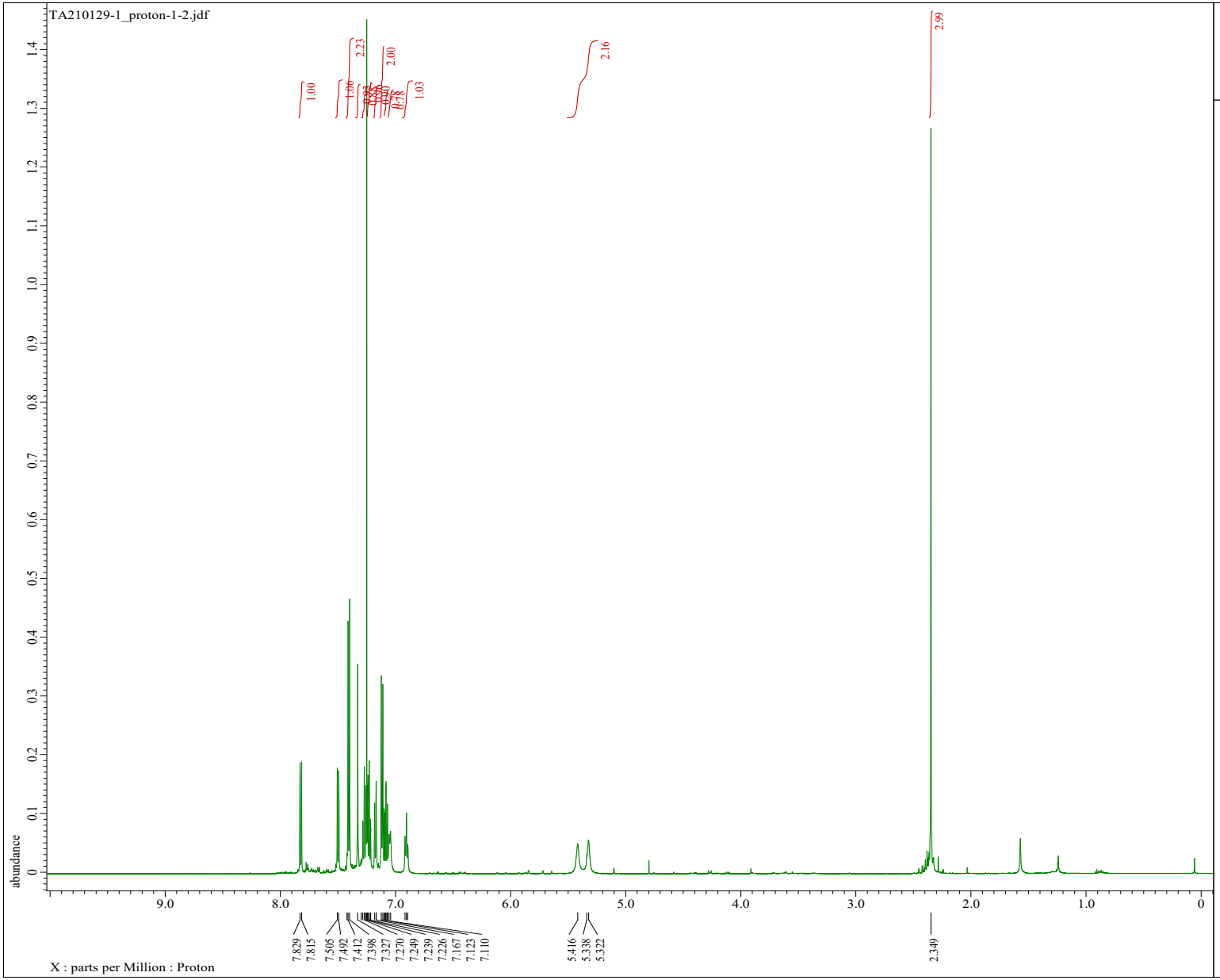
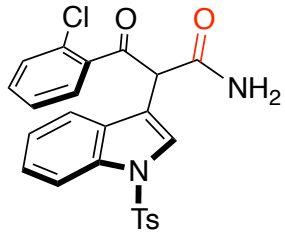


JEOL

Filename	= TA210129-1_proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210129-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JAN-2021 21:22:53
Revision_Time	= 29-JAN-2021 21:25:57
Comment	= 2Cl-Bz-acetonitrile
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.2[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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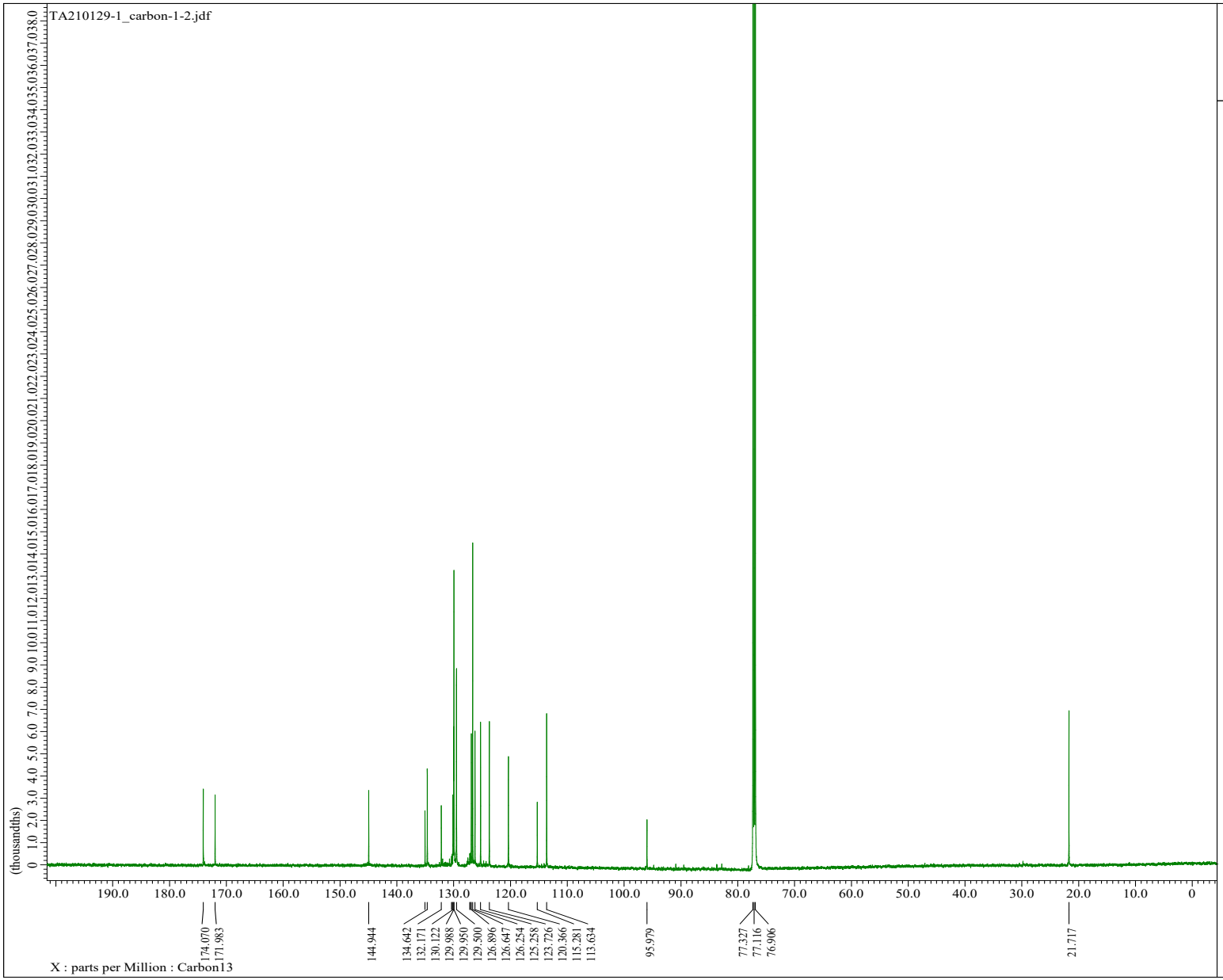
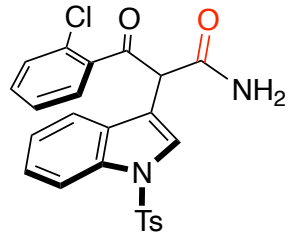


Filename	= TA210129-1_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210129-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JAN-2021 21:27:
Revision_Time	= 30-JAN-2021 09:04:
Comment	= 2Cl-Bz-acetonitril
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
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	= 4500
Total_Scans	= 4500
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.4[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_Templ	= 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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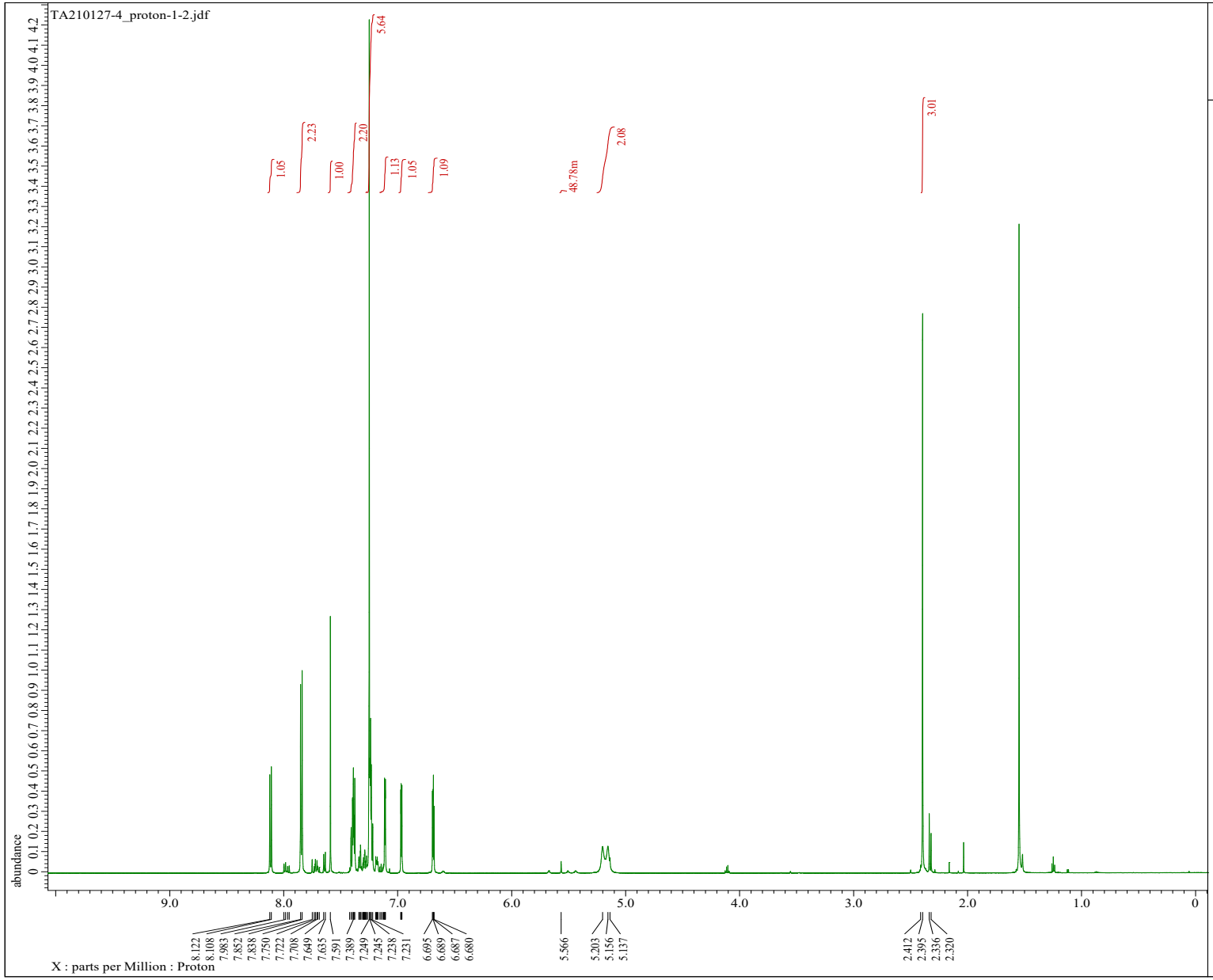
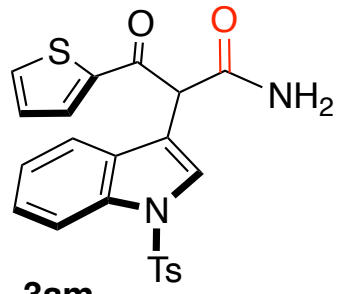


JEOL

Filename	= TA210127-4_proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210127-4
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JAN-2021 21:12:11
Revision_Time	= 27-JAN-2021 21:12:43
Comment	= thienyl
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 21[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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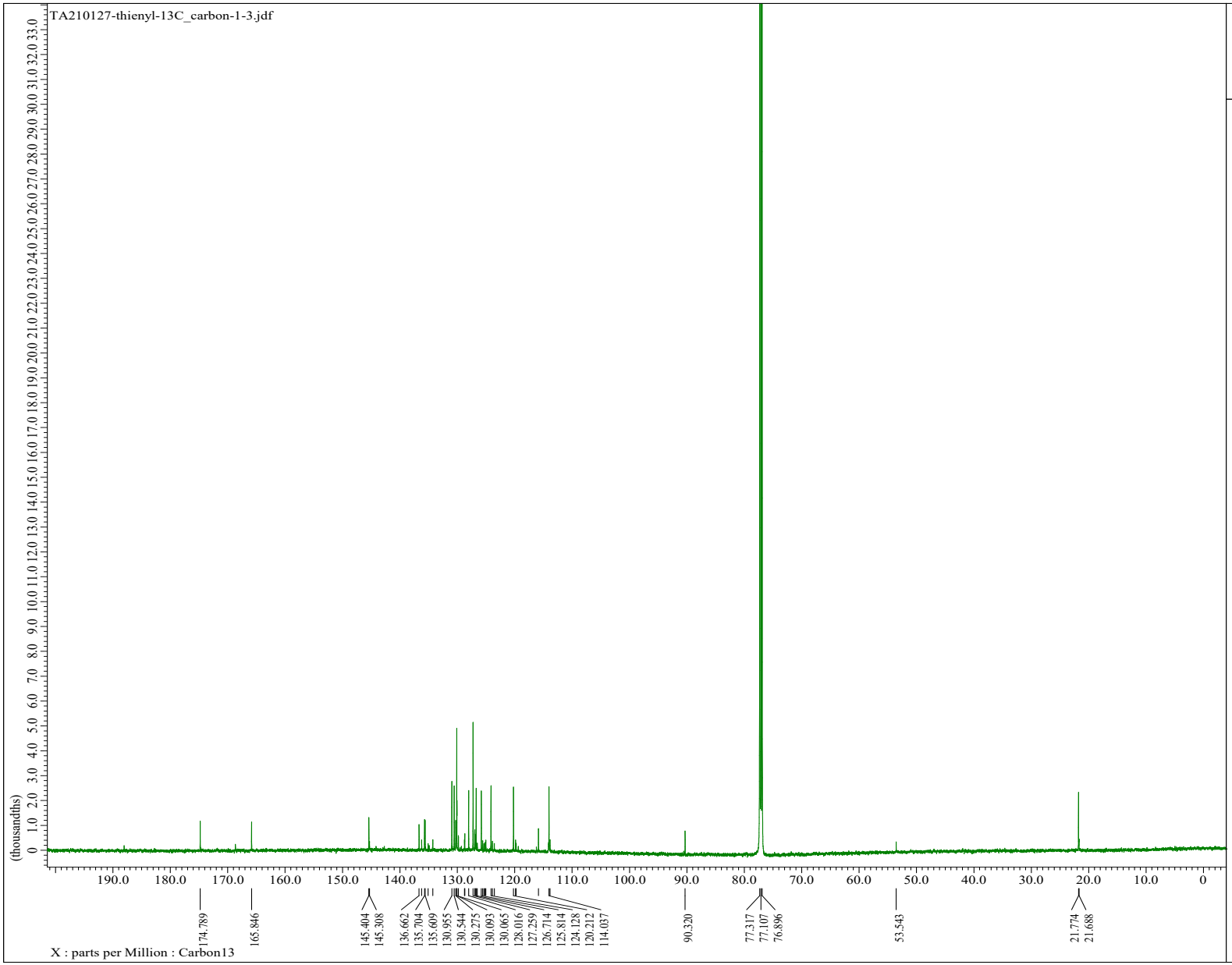
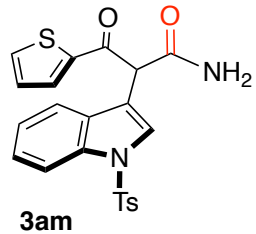


JEOL

Filename	= TA210127-thienyl-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210127-thienyl-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-JAN-2021 20:11:
Revision_Time	= 28-JAN-2021 21:53:
Comment	= thienyl
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	= 3084
Total_Scans	= 3084
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.6[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_Templ	= 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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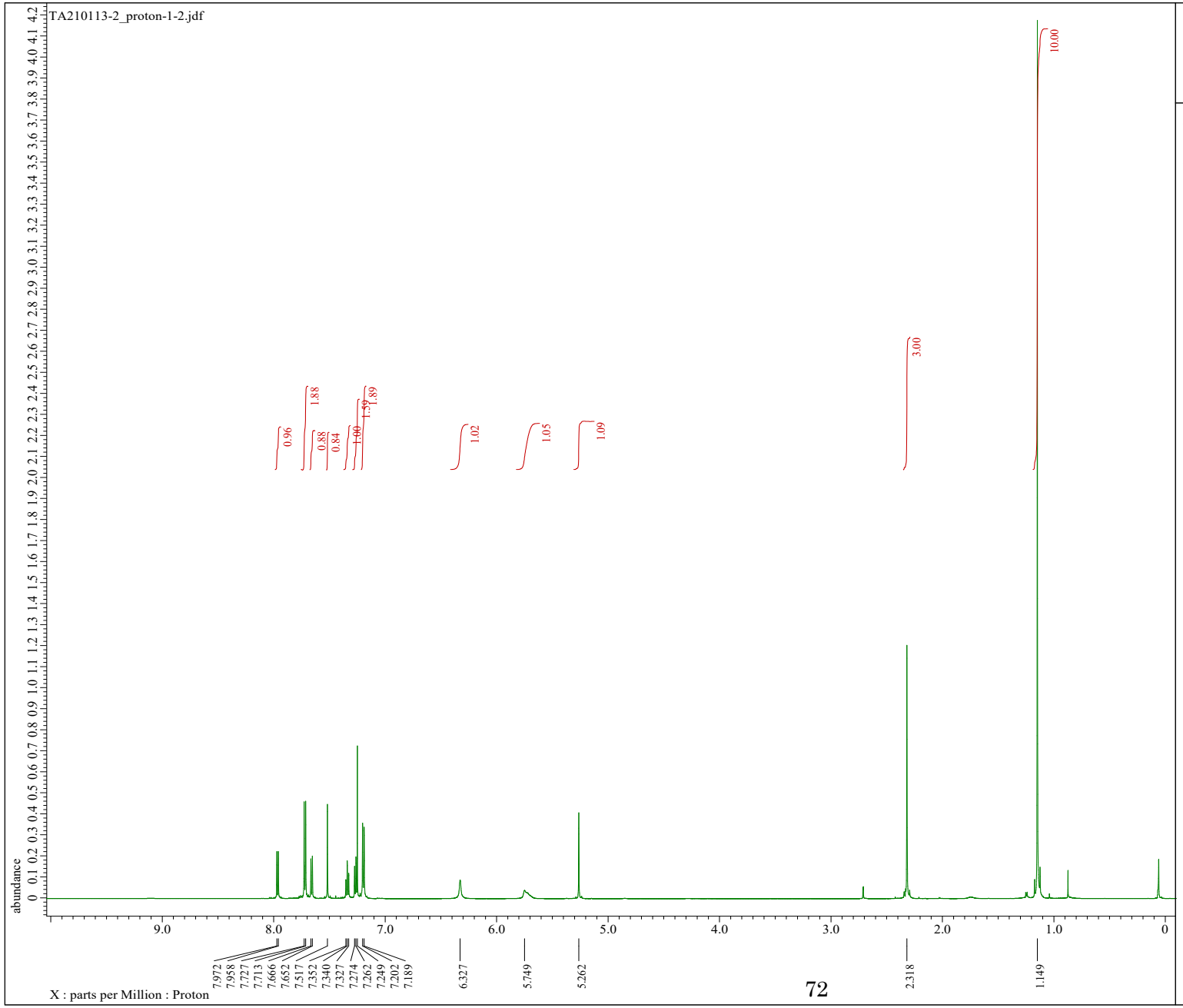
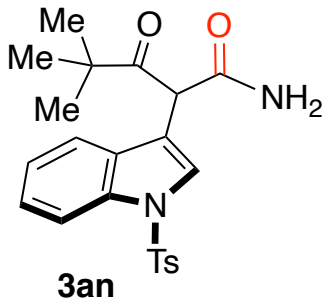


Filename	= TA210113-2_proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210113-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-JAN-2021 20:36:14
Revision_Time	= 13-JAN-2021 20:40:07
Comment	= Piv
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 5[s]
Recvr_Gain	= 26
Temp_Get	= 19.8[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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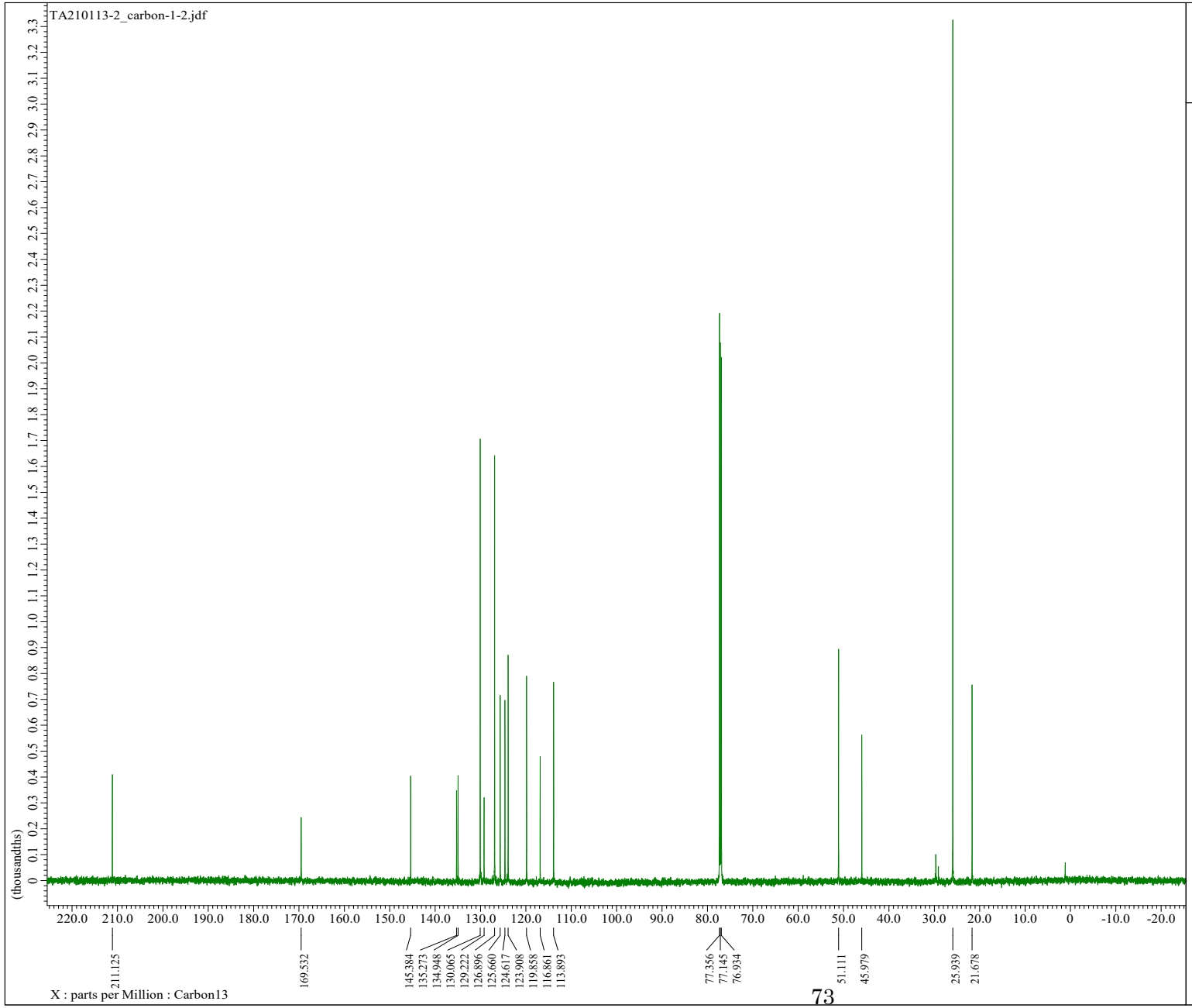
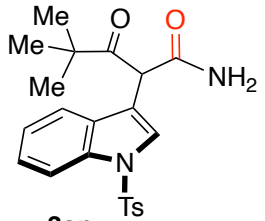
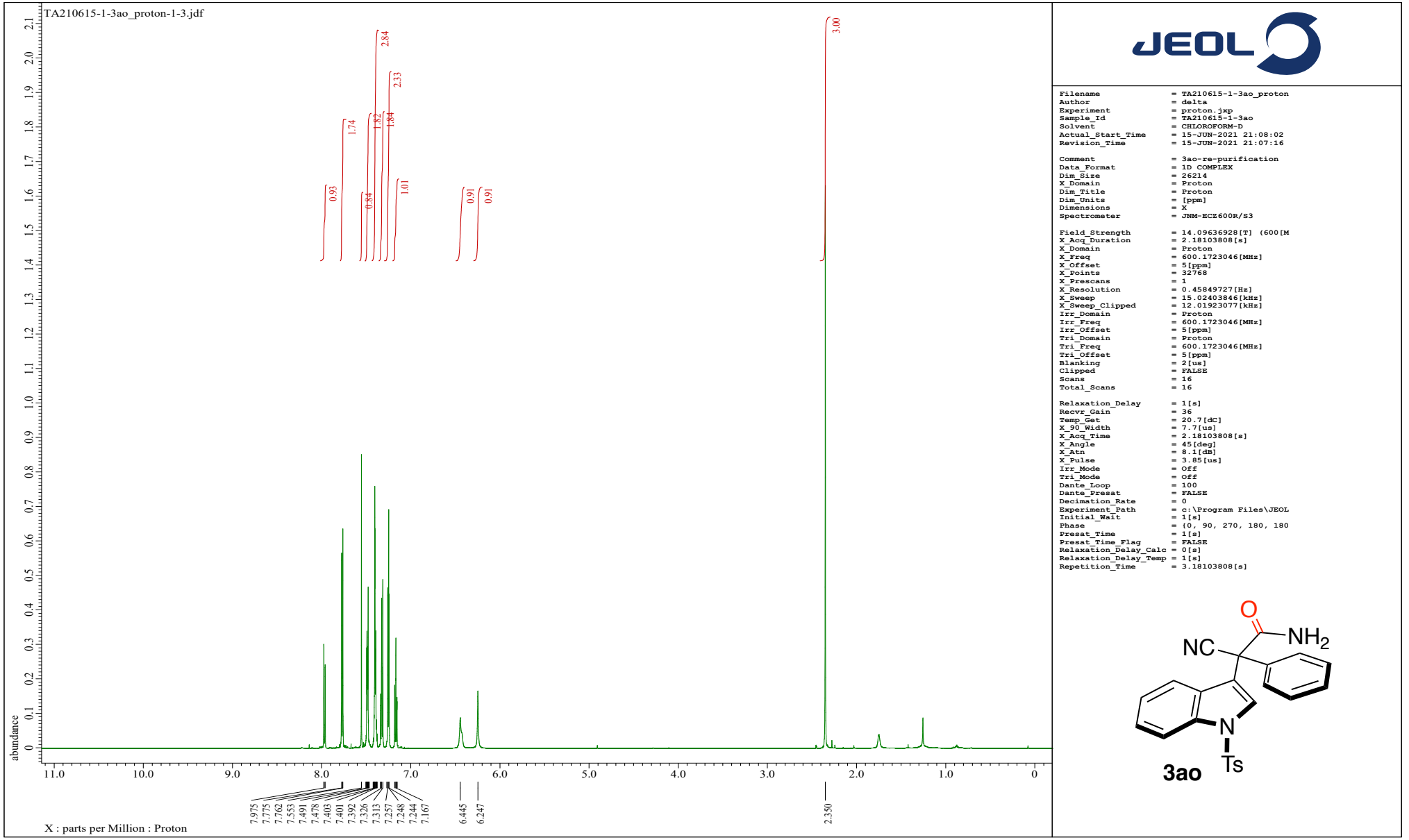


Filename	= TA210113-2_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210113-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-JAN-2021 20:40:
Revision_Time	= 13-JAN-2021 21:23:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
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	= 1351
Total_Scans	= 1351
Relaxation_Delay	= 1[s]
Recvr_Gain	= 26
Temp_Get	= 19.7[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_Templ	= 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]



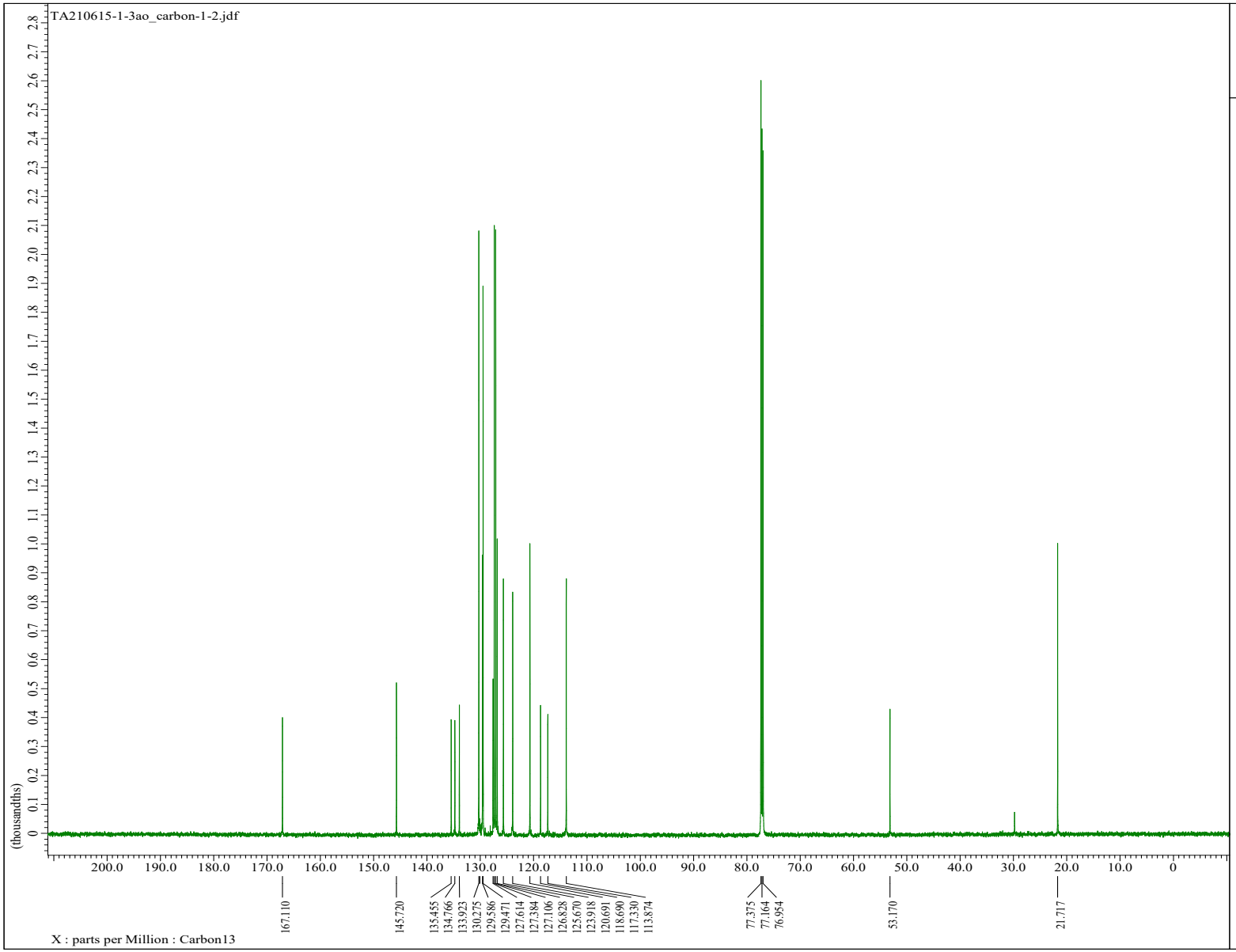
3an



JEOL

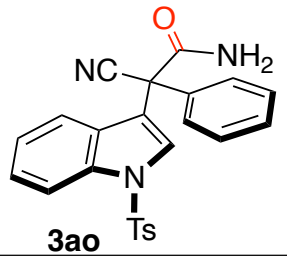
Filename	= TA210615-1-3ao_proton
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210615-1-3ao
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JUN-2021 21:08:02
Revision_Time	= 15-JUN-2021 21:07:16
Comment	= 3ao-re-purification
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= 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	= 20.7[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]

3ao

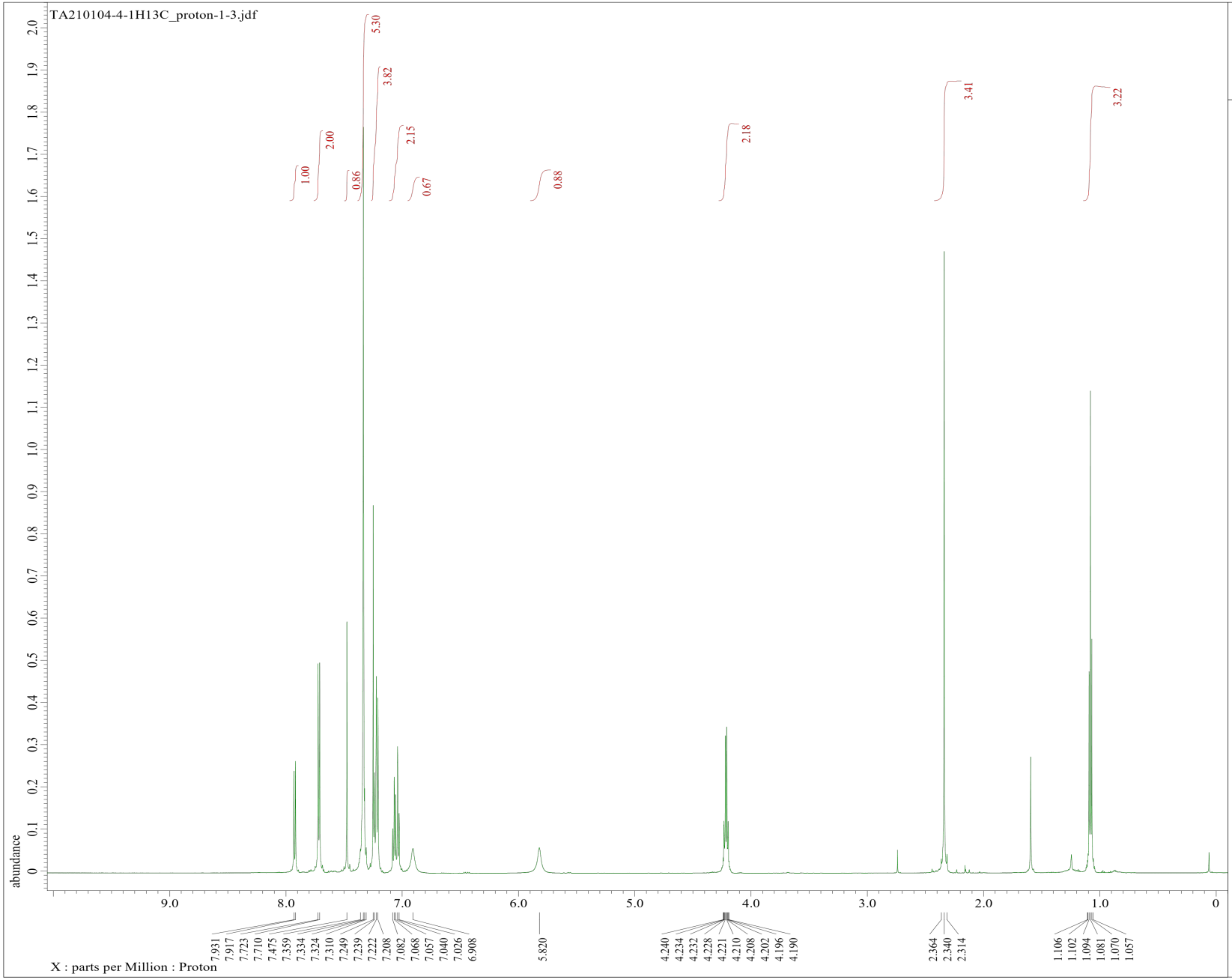


JEOL

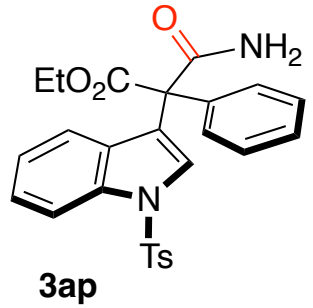
Filename	= TA210615-1-3ao_car
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210615-1-3ao
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JUN-2021 21:09:
Revision_Time	= 16-JUN-2021 09:23:
Comment	= 3ao-repurification
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
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	= 1736
Total_Scans	= 1736
Relaxation_Delay	= 2[s]
Recvr_Gain	= 26
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	= 7.2368421[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
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]



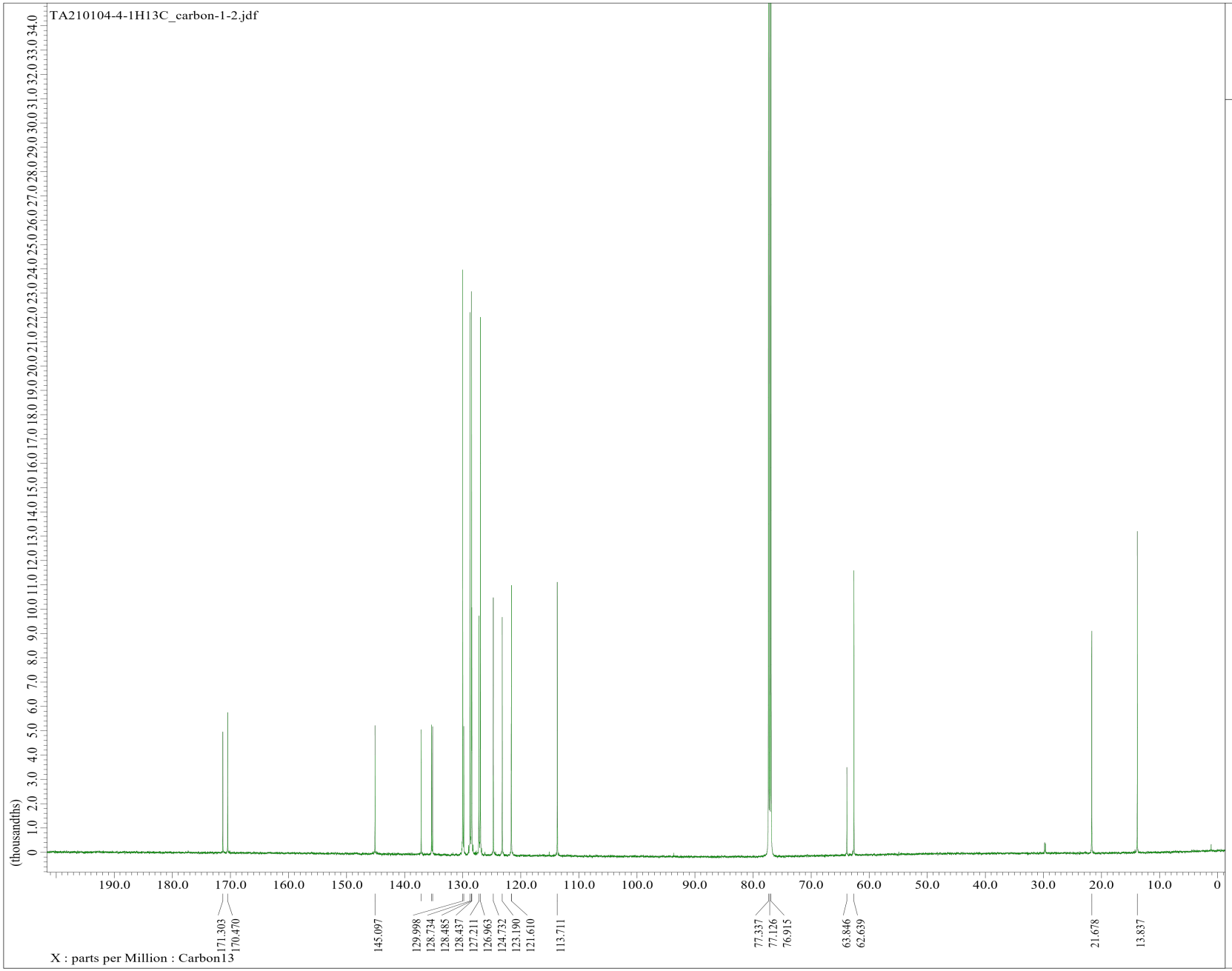
3ao



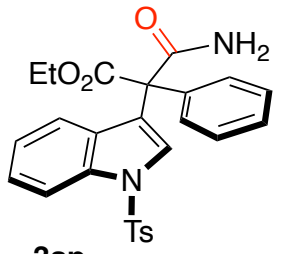

```
Filename                = TA210104-4-1H13C_prot
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = TA210104-4-1H13C
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  5-JAN-2021 02:20:16
Revision_Time           =  5-JAN-2021 08:27:37

Comment                 = single_pulse-Ph-CN-CO
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
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          = 1.4548992[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.68733284[Hz]
X_Sweep                 = 11.26126126[kHz]
X_Sweep_Clipped         = 9.00900901[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        = 5[s]
Recvr_Gain              = 36
Temp_Get                = 21.3[dC]
X_90_Width              = 9.5[us]
X_Acq_Time              = 1.4548992[s]
X_Angle                 = 45[deg]
X_Atn                   = 8.1[dB]
X_Pulse                 = 4.75[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         = 6.4548992[s]
```



3ap



Filename	= TA210104-4-1H13C_c
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210104-4-1H13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JAN-2021 02:25:
Revision_Time	= 5-JAN-2021 08:11:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-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	= 10000
Total_Scans	= 10000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.6[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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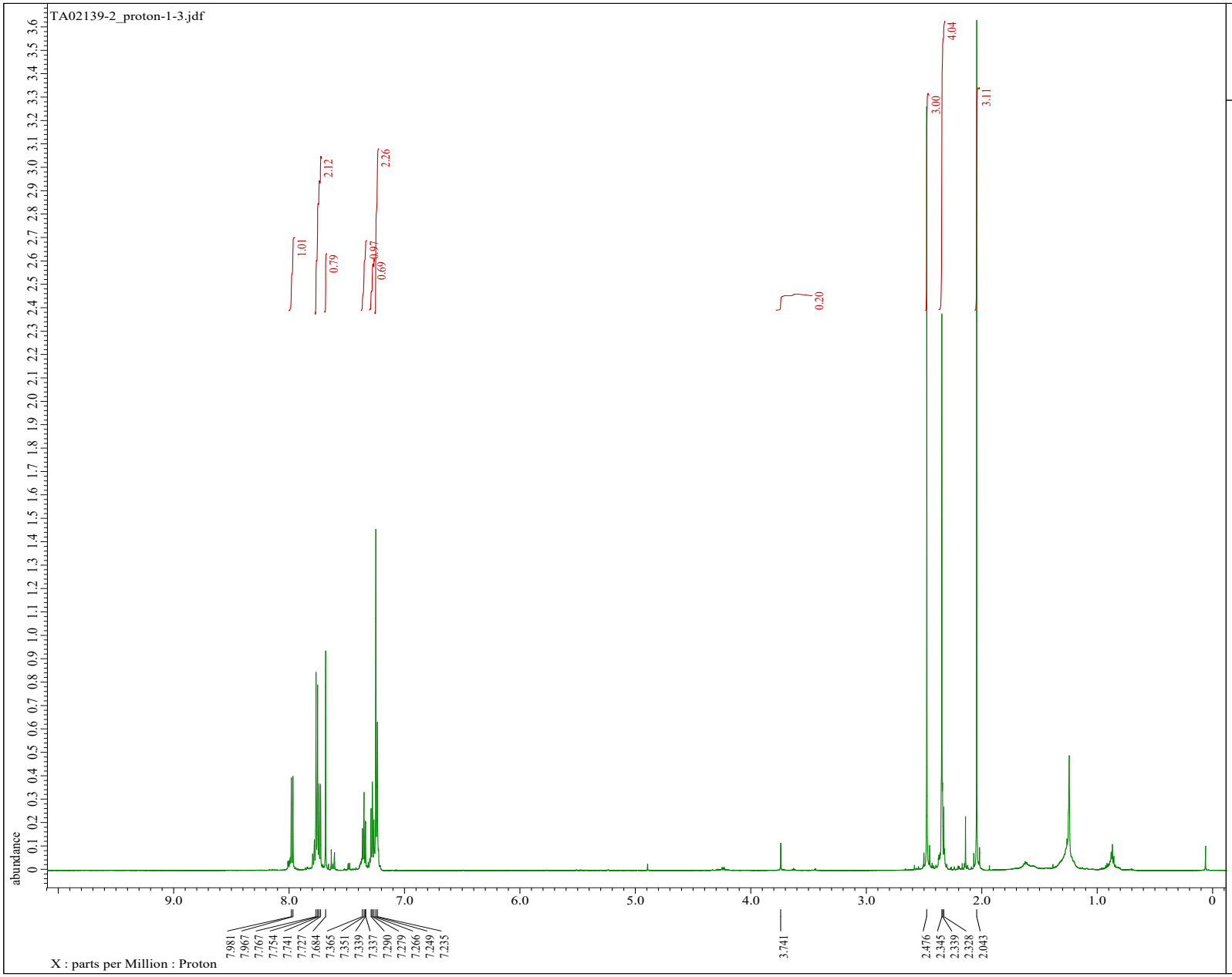
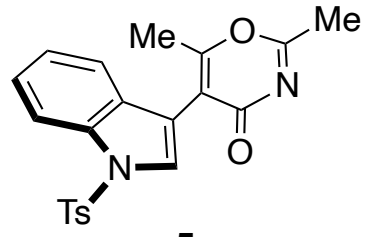


Filename	= TA02139-2_proton-1-3.
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA02139-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-DEC-2020 20:31:17
Revision_Time	= 14-DEC-2020 20:45:30
Comment	= single_pulse-Ac-indol
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.45227776[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68857351[Hz]
X_Sweep	= 11.28158845[kHz]
X_Sweep_Clipped	= 9.02527076[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.6[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.45227776[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.45227776[s]



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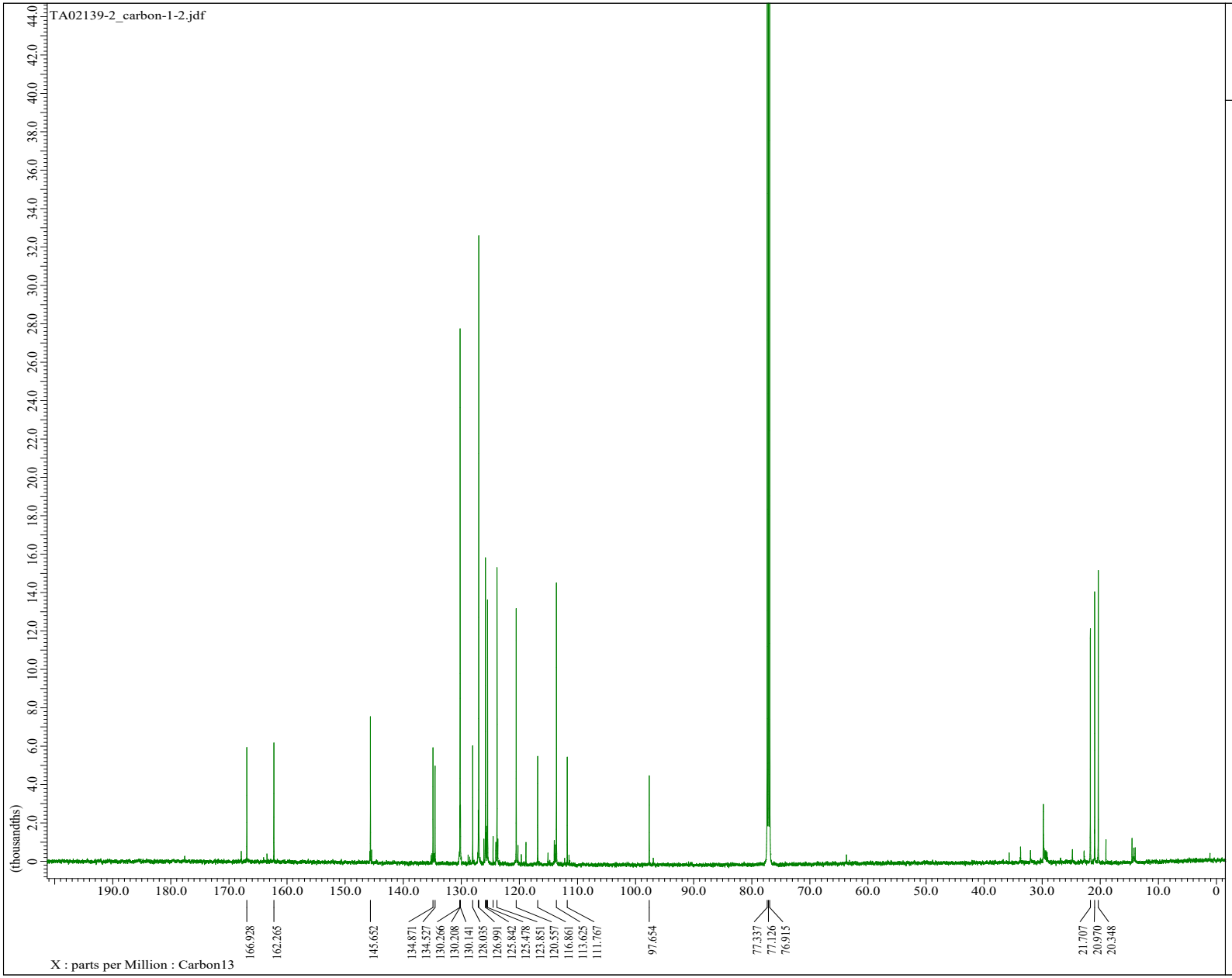
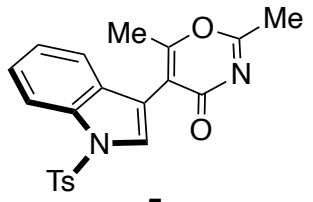
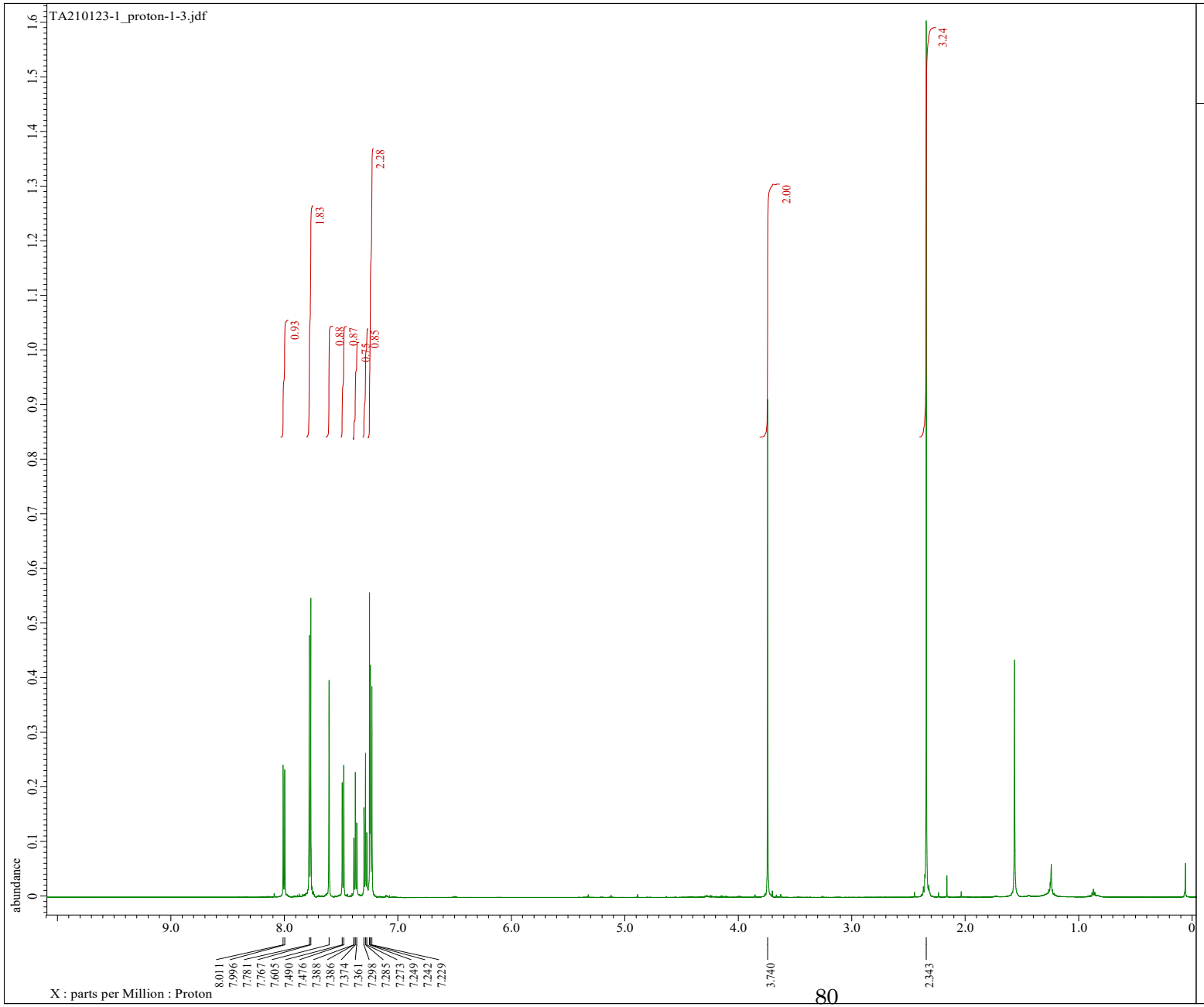


JEOL

Filename	= TA02139-2_carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA02139-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-DEC-2020 20:35:
Revision_Time	= 14-DEC-2020 21:17:
Comment	= single pulse decou
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	= 1300
Total_Scans	= 1300
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.8[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]



5



Filename	= TA210123-1_proton-1-3
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210123-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JAN-2021 17:05:49
Revision_Time	= 23-JAN-2021 17:17:14
Comment	= 3-CH2CN
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.7[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]

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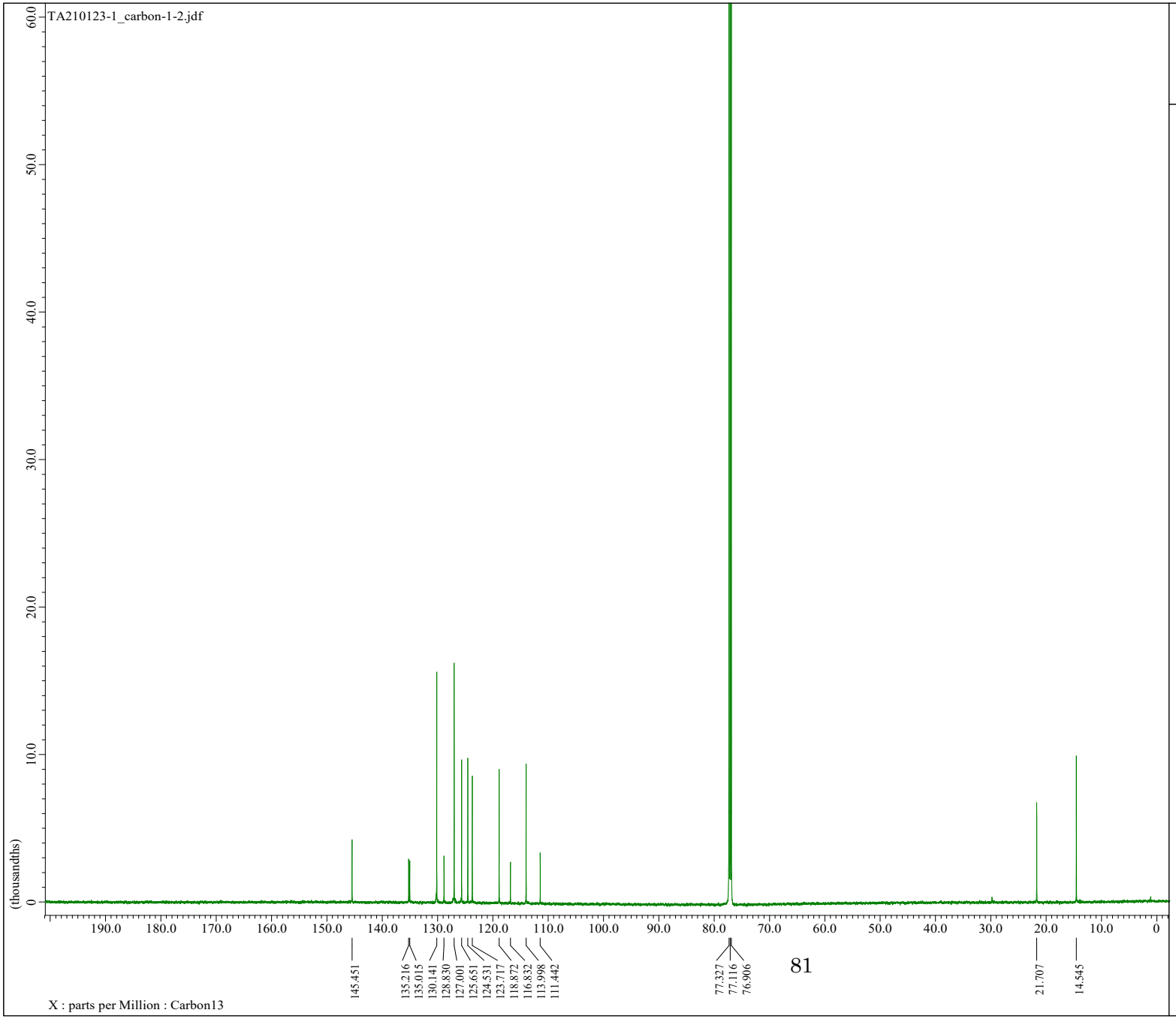
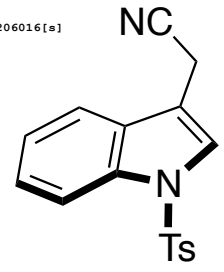


JEOL

Filename	= TA210123-1_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210123-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JAN-2021 19:11:
Revision_Time	= 23-JAN-2021 20:09:
Comment	= 3-CH2CN
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	= 1820
Total_Scans	= 1820
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.6[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_Templ	= 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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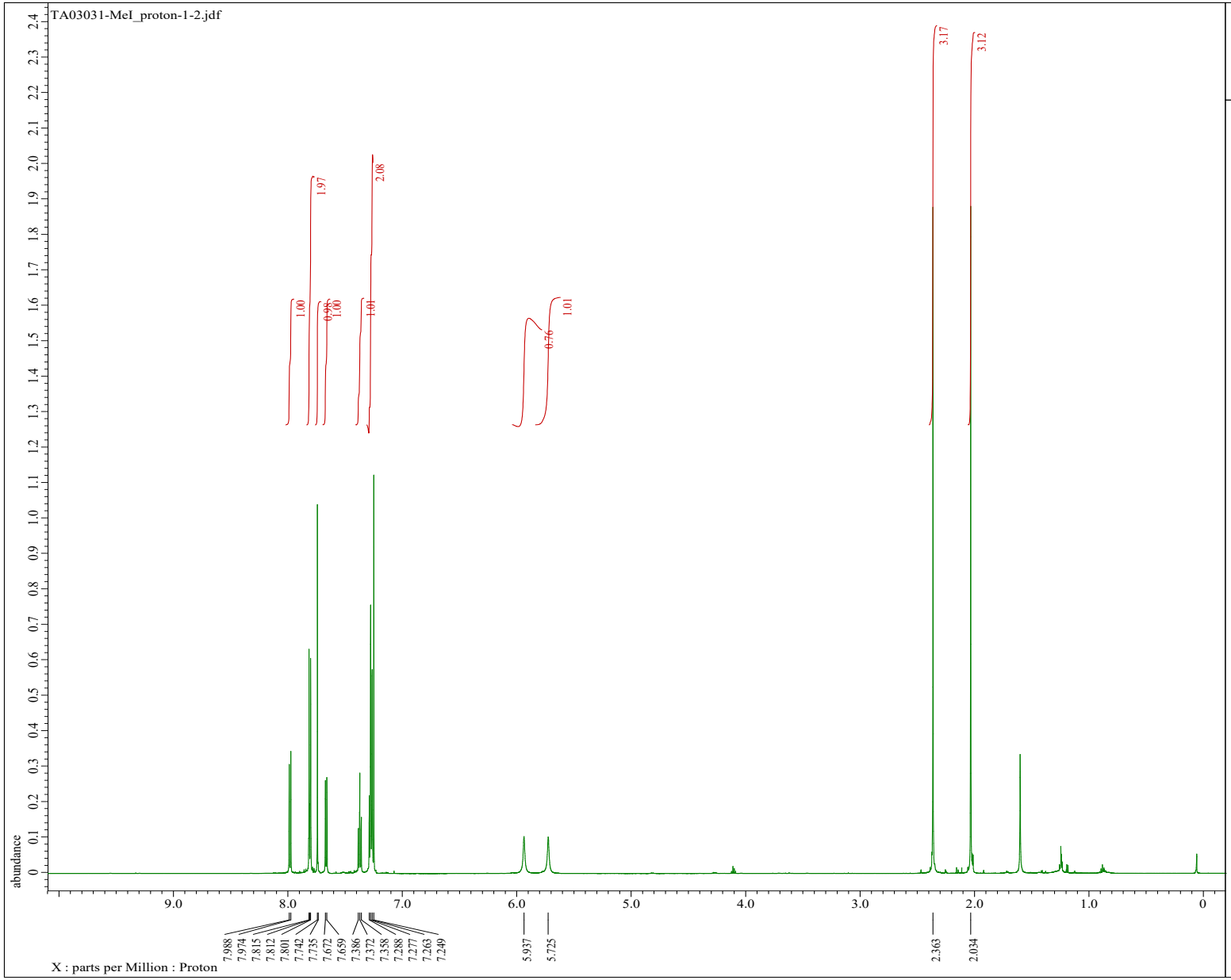
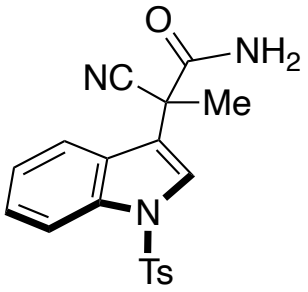


JEOL

Filename	= TA03031-MeI_proton-1-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA03031-MeI
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2021 20:34:21
Revision_Time	= 22-JAN-2021 20:36:41
Comment	= MeI
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.2[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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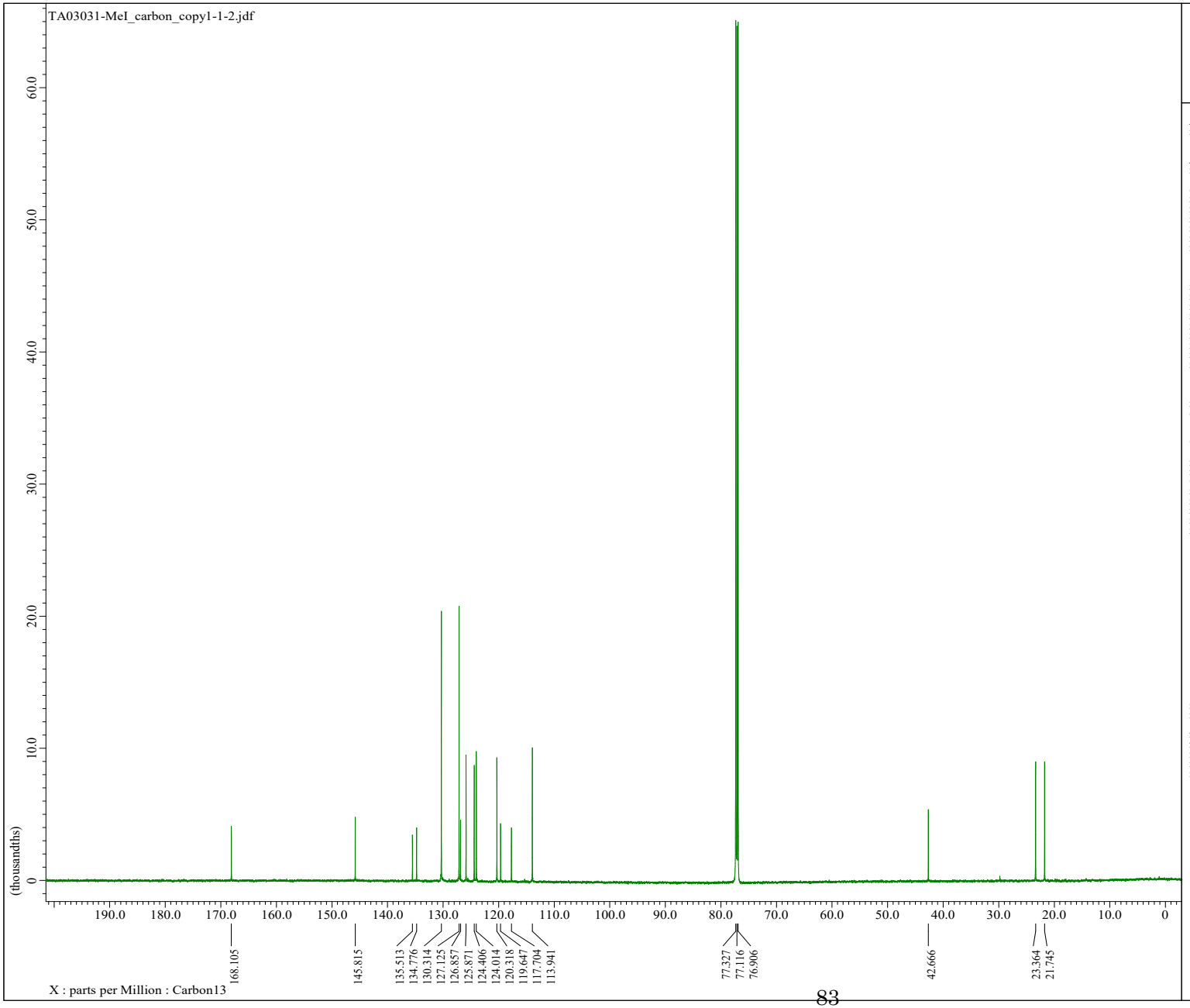
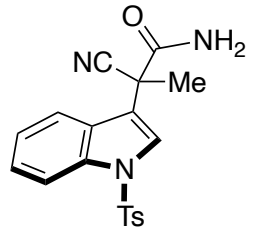


JEOL

Filename	= TA03031-MeI_carbon
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA03031-MeI
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2021 20:38:
Revision_Time	= 22-JAN-2021 21:50:
Comment	= MeI
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
Incomplete_Copy	= TRUE
Scans	= 2193
Total_Scans	= 2193
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 21[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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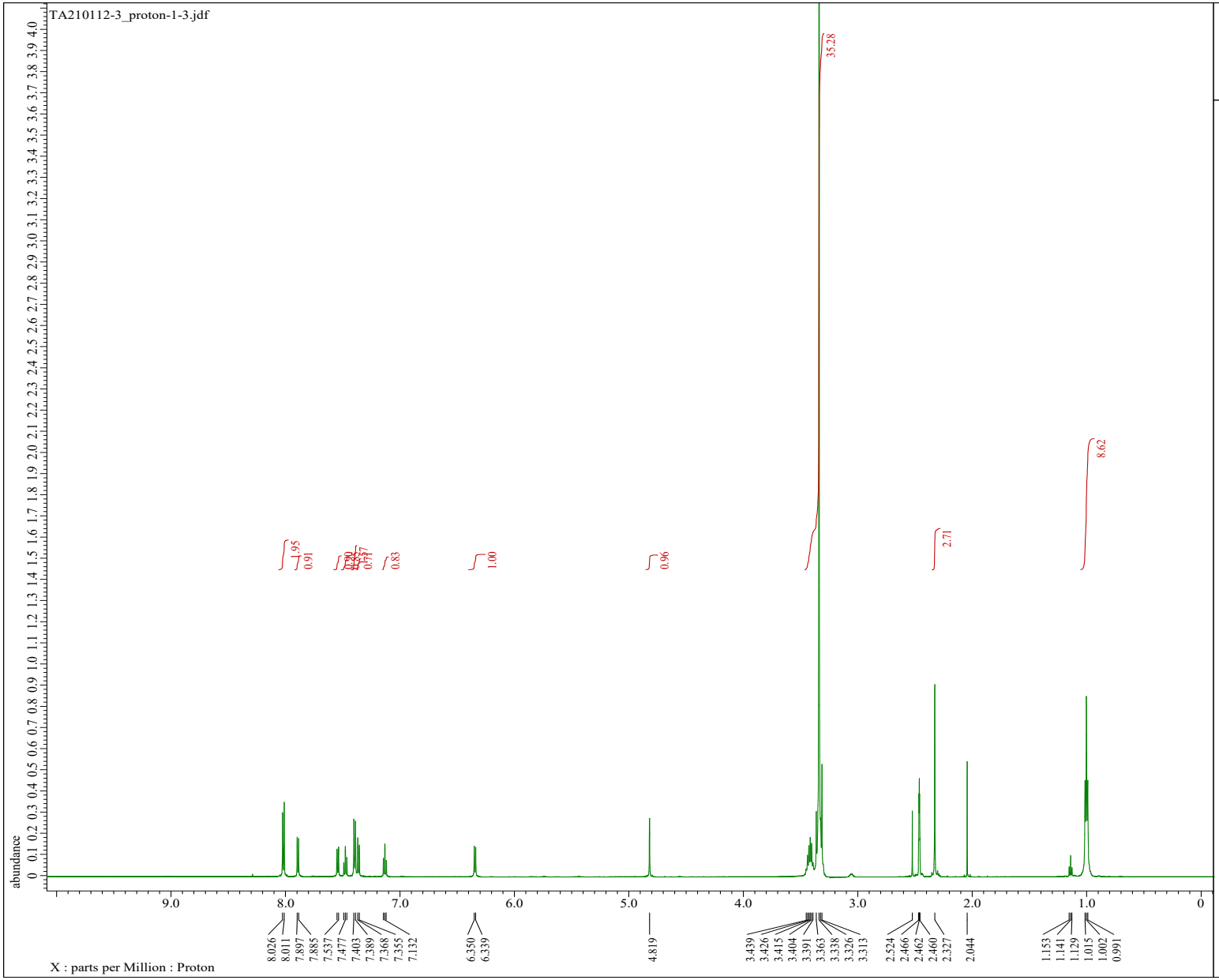
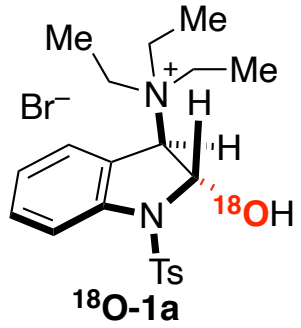


JEOL

Filename	= TA210112-3_proton-1-3
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210112-3
Solvent	= DMSO-D6
Actual_Start_Time	= 12-JAN-2021 20:53:04
Revision_Time	= 13-JAN-2021 09:10:40
Comment	= 18O-HITAB-DMSO
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 18.5[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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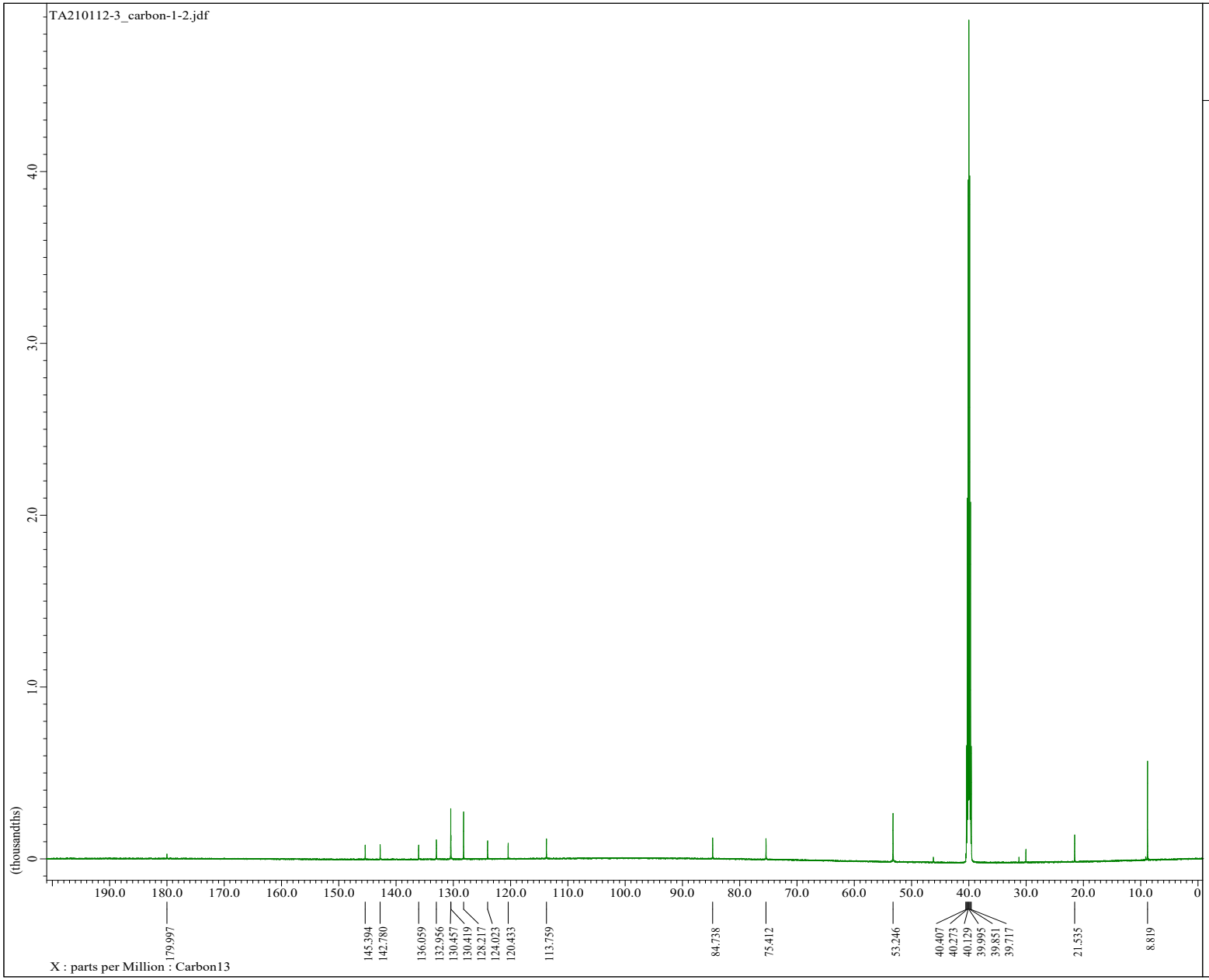
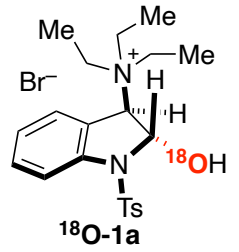


JEOL

Filename	= TA210112-3_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210112-3
Solvent	= DMSO-D6
Actual_Start_Time	= 12-JAN-2021 20:57:
Revision_Time	= 13-JAN-2021 09:17:
Comment	= single pulse decou
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	= 4000
Total_Scans	= 4000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 26
Temp_Get	= 19[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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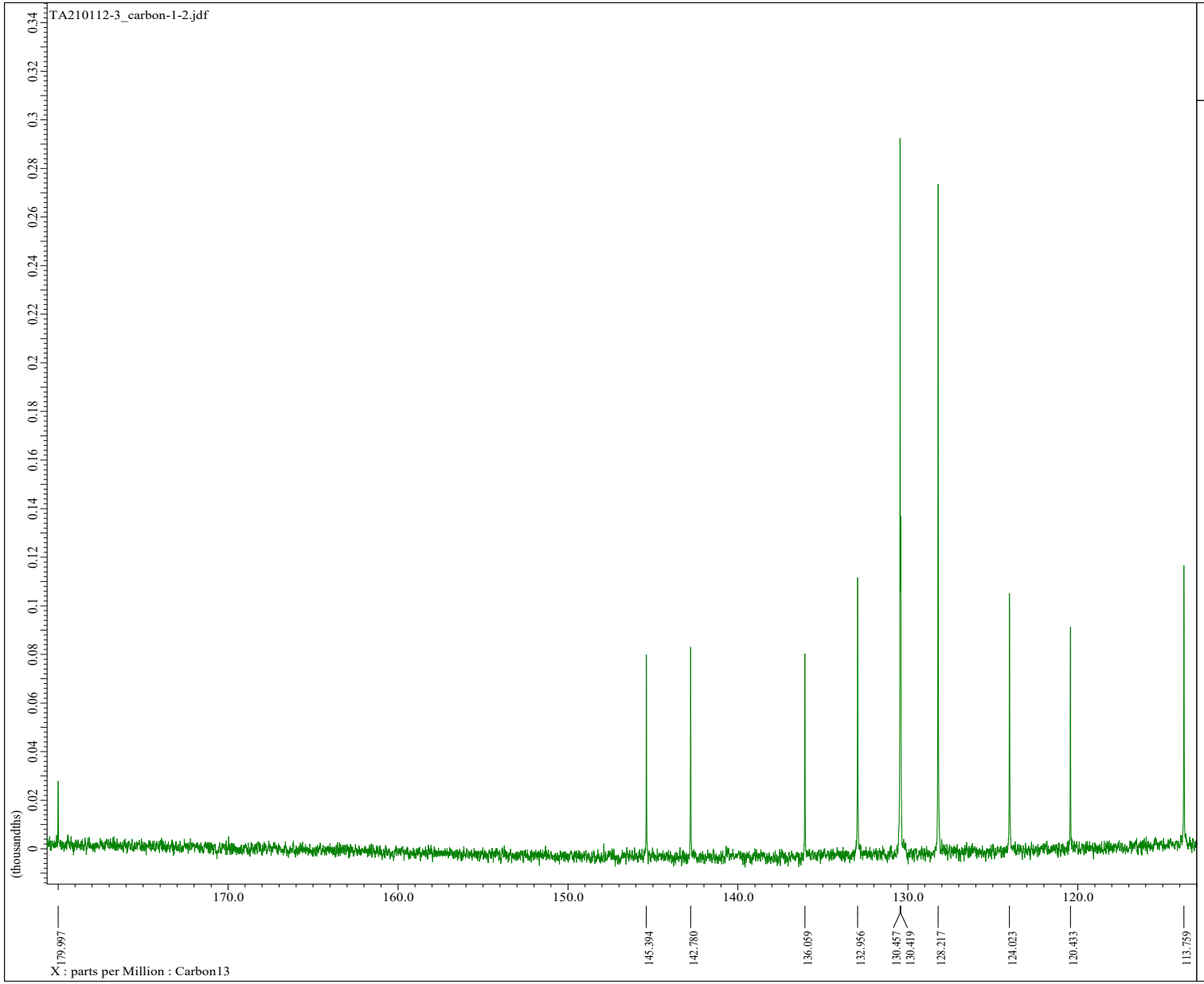
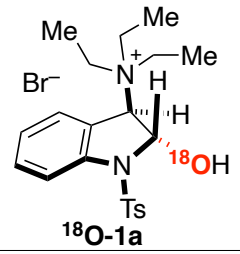


JEOL

Filename	= TA210112-3_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210112-3
Solvent	= DMSO-D6
Actual_Start_Time	= 12-JAN-2021 20:57:
Revision_Time	= 13-JAN-2021 09:17:
Comment	= single pulse decou
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	= 4000
Total_Scans	= 4000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 26
Temp_Get	= 19[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_Templ	= 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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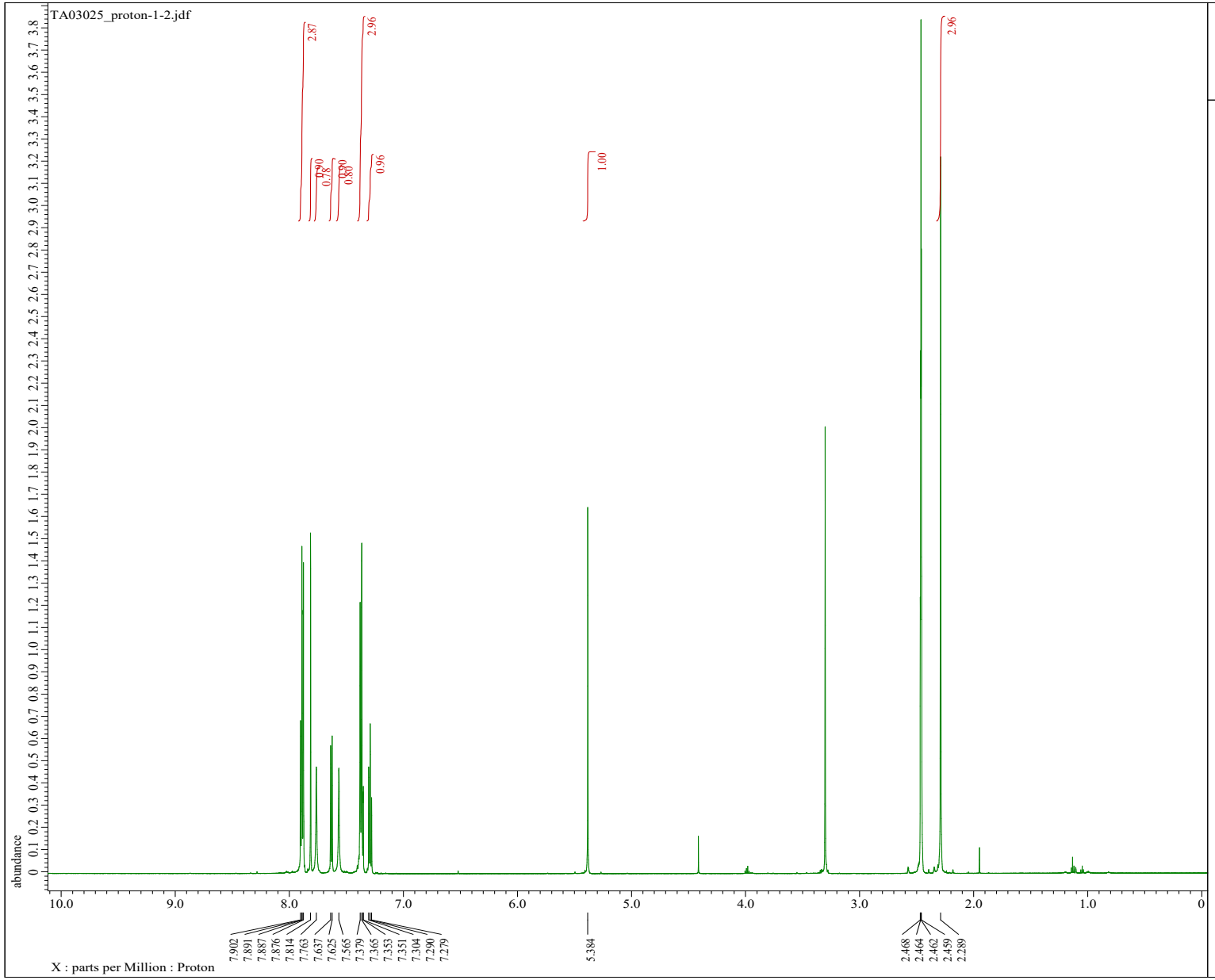
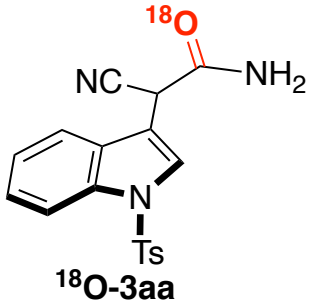


JEOL

Filename	= TA03025_proton-1-2.jd
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA03025
Solvent	= DMSO-D6
Actual_Start_Time	= 14-JAN-2021 13:28:09
Revision_Time	= 14-JAN-2021 13:27:30
Comment	= 18O-indolylacetamide
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.4548992[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
X_Sweep_Clipped	= 9.00900901[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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.4[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.4548992[s]



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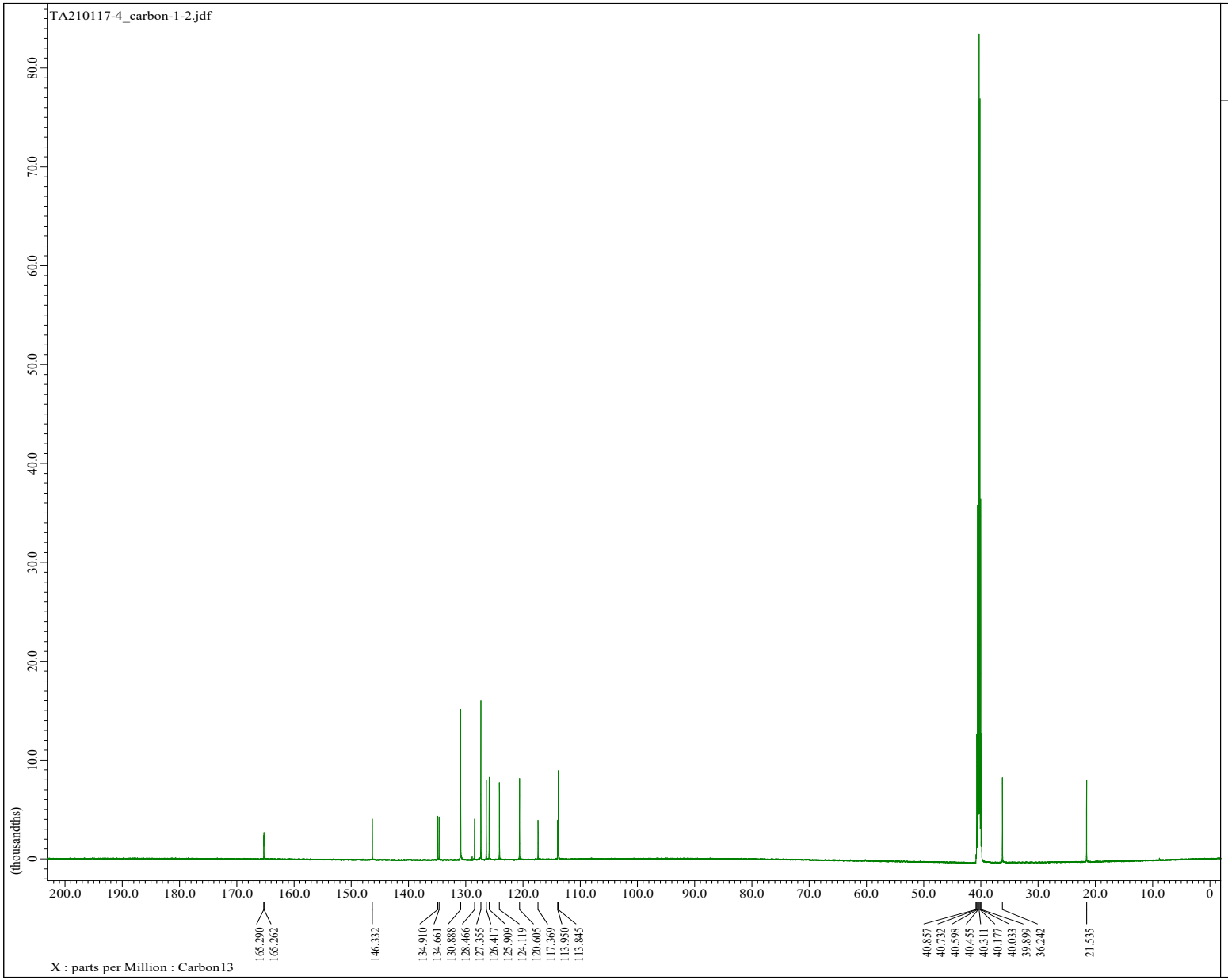
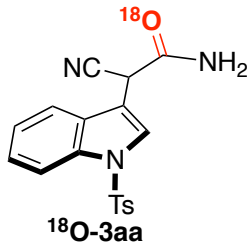


JEOL

Filename	= TA210117-4_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210117-4
Solvent	= DMSO-D6
Actual_Start_Time	= 18-JAN-2021 05:31:
Revision_Time	= 18-JAN-2021 08:19:
Comment	= 4F-keto-enol-DMSO
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	= 5000
Total_Scans	= 5000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 60[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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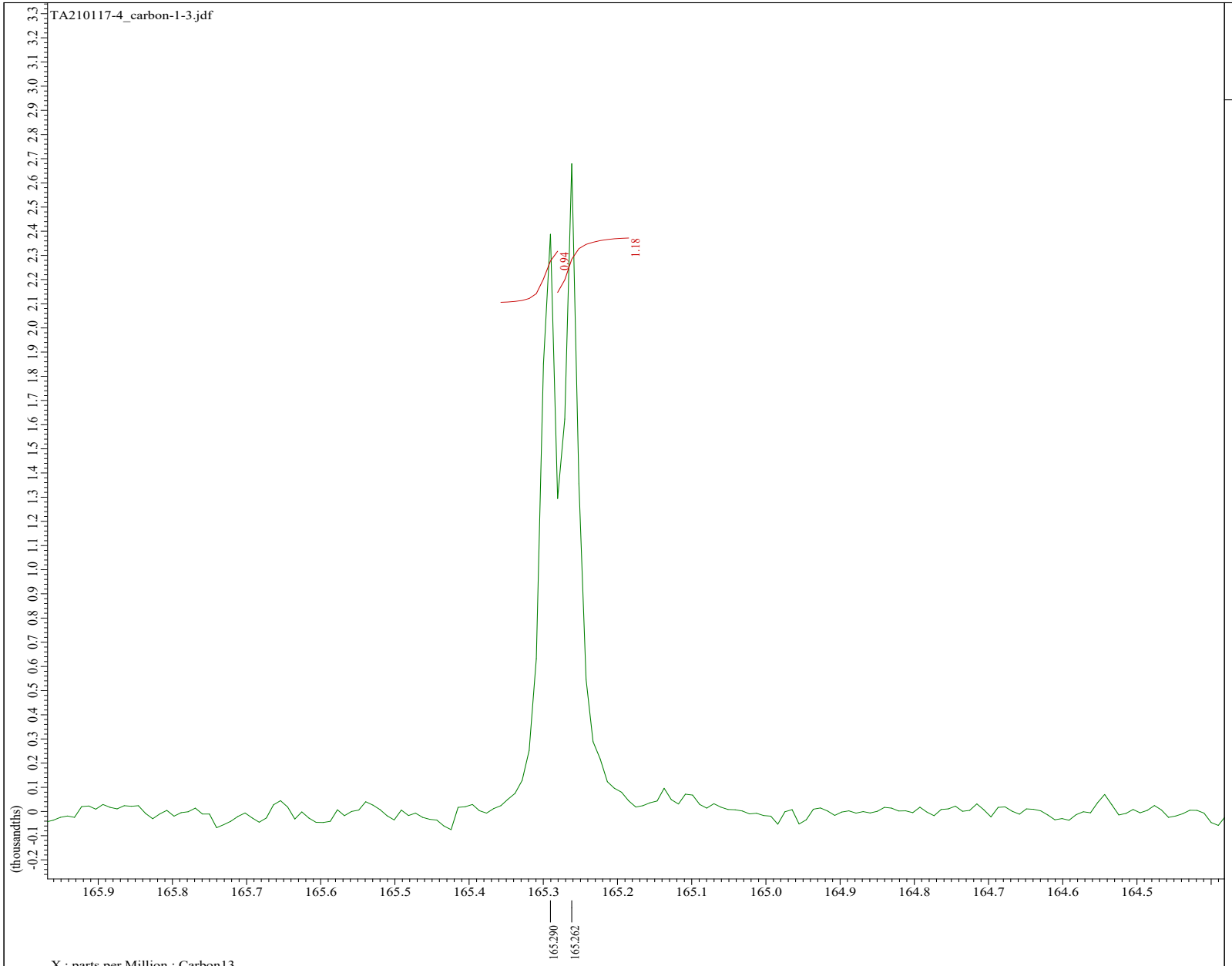
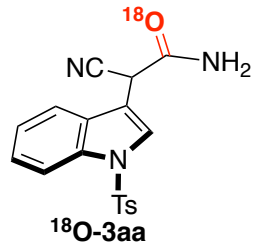


JEOL

Filename	= TA210117-4_carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= TA210117-4
Solvent	= DMSO-D6
Actual_Start_Time	= 18-JAN-2021 05:31:
Revision_Time	= 19-JAN-2021 20:44:
Comment	= 4F-keto-enol-DMSO
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	= 5000
Total_Scans	= 5000
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 60[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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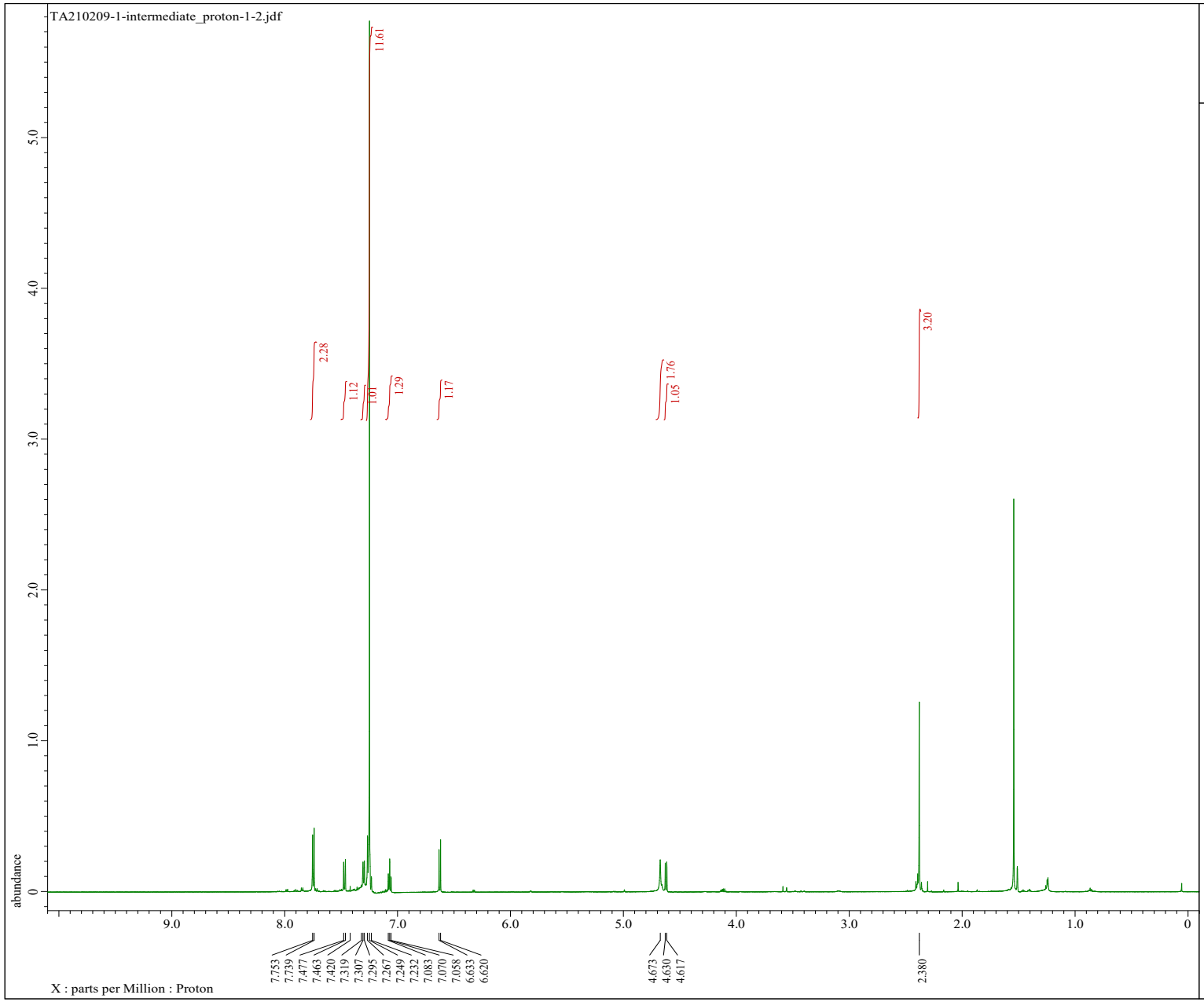
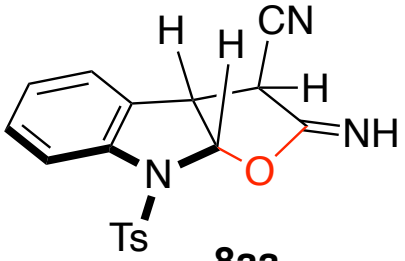


JEOL

Filename	= TA210209-1-intermedia
Author	= delta
Experiment	= proton.jxp
Sample_Id	= TA210209-1-intermedia
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-FEB-2021 20:31:43
Revision_Time	= 9-FEB-2021 20:32:46
Comment	= intermediate
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 1.09051904[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.91699454[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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 20.3[dC]
X_90_Width	= 9.5[us]
X_Acq_Time	= 1.09051904[s]
X_Angle	= 45[deg]
X_Atn	= 8.1[dB]
X_Pulse	= 4.75[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	= 6.09051904[s]



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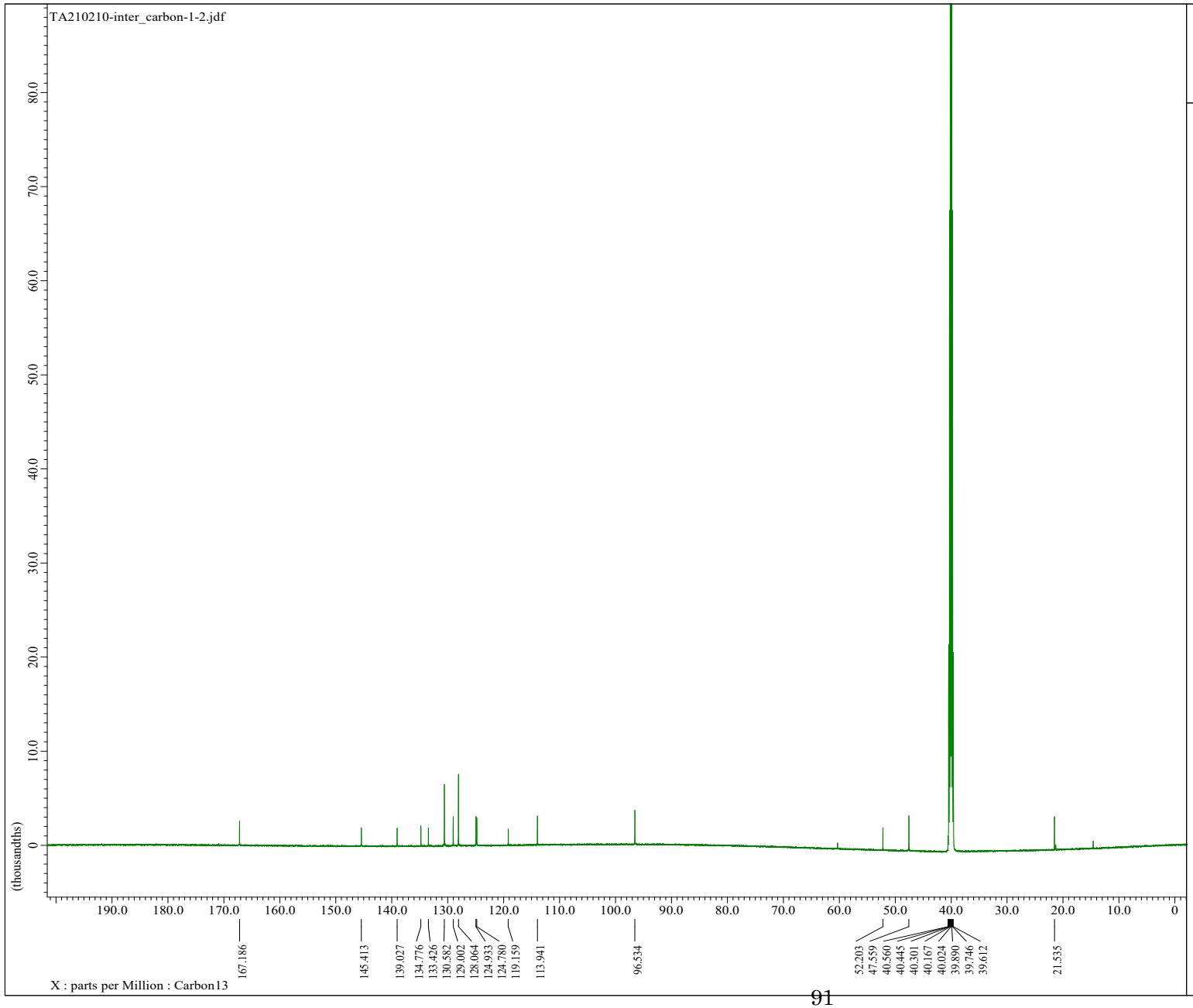
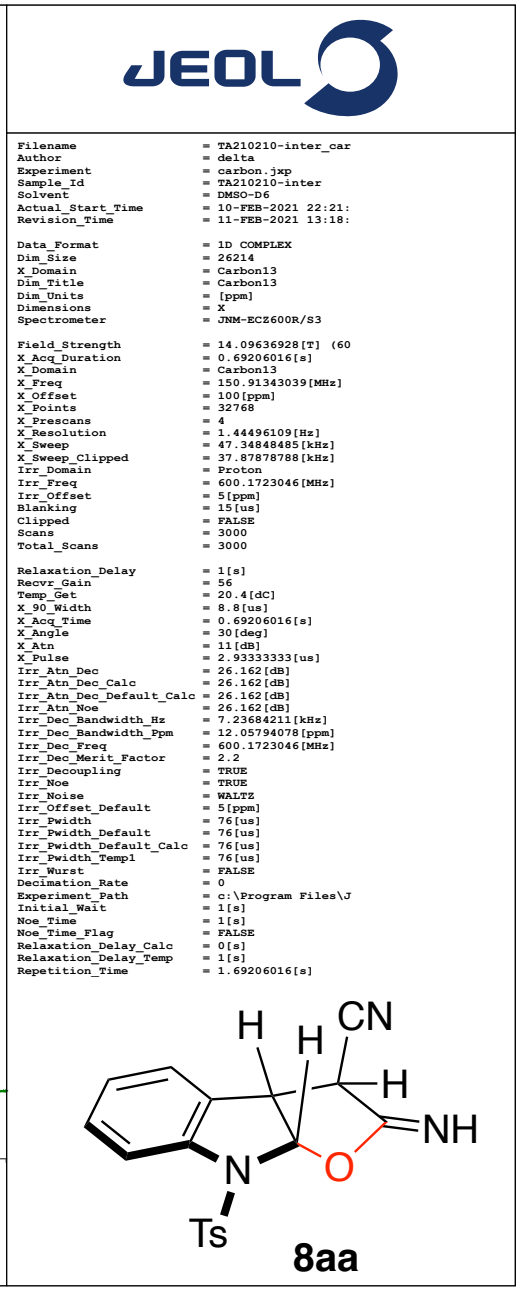

TA210210-inter_carbon-1-2.jdf
(thousandths)
X : parts per Million : Carbon13
167.186
145.413
139.027
134.776
133.426
130.582
129.002
128.064
124.933
124.780
119.159
113.941
96.534
52.203
47.559
40.560
40.445
40.301
40.167
40.024
39.890
39.746
39.612
21.535


JEOL
Filename = TA210210-inter_car
Author = delta
Experiment = carbon.jxp
Sample_Id = TA210210-inter
Solvent = DMSO-D6
Actual_Start_Time = 10-FEB-2021 22:21:
Revision_Time = 11-FEB-2021 13:18:
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (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 = 3000
Total_Scans = 3000
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 20.4[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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