Electronic Supplementary Material (ESI) for ChemComm.

A metal-, oxidant-, and fluorous solvent-free synthesis of α-indolylketones enabled by umpolung strategy

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SUPPORTING INFORMATION

Contents

Experimental Section

1. General Experimental

Mass-spectrometry

High-resolution mass spectra were recorded with a JEOL JMS-T100LP mass spectrometers.

NMR spectroscopy

NMR experiments were performed with a JEOL JNM-ECA500 spectrometer operating at 500 MHz and 125 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 (Silica Gel 63–210 mesh, Kanto Chemical Co., Ltd.).

Starting materials

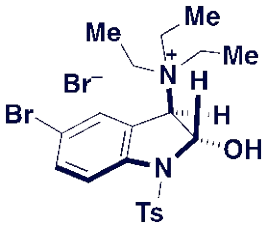
The ROBIN (2-RO-3-bromoindoline, **1a**), and 3-methoxyindole (3-MeOIN, **5**) were prepared by reported methods.[S1] 3-bromo-2-hydroxyindoline **1b**, 3-bromoindole **2**, and HITABs (2-hydroxyindoline-3-triethylammonium bromides, **3**) were prepared by reported methods.[S2] DiMeOIN (2,3-dimethoxyindoline, **4**) was prepared by reported methods.[S3] Enamines **6** were prepared by reported methods.[S4]

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.

2. Experimental Procedure

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

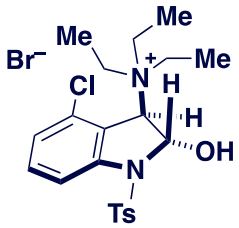
trans-2-Hydroxy-5-bromo-1-tosylindoline-3-ammonium bromide (3d)



To a solution of 5-bromo-1-tosylindole (701 mg, 2 mmol) and H_2O (0.36 mL, 20 mmol) in acetone (20 mL) was added NBS (392 mg, 2.2 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material as indicated by TLC. Et_3N (0.31 mL, 2.2 mmol) was added to the mixture and stirred further 1 h. The resulting precipitate was separated by filtration, washed with acetone, and dried *in vacuo* to give **3d** (746.1 mg, 68% yield).

746.1 mg, 68% yield. colorless solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ: 8.01 (d, J = 8.6 Hz, 2H), 7.93 (d, J = 8.0 Hz, 1H), 7.70 (s, 1H), 7.66 (dd, J = 8.6, 1.8 Hz, 1H), 7.41(d, J = 8.0 Hz, 2H), 7.32 (d, J = 9.2 Hz, 1H), 6.35 (d, J = 7.4 Hz, 1H), 4.83 (s, 1H), 3.33–3.46 (m, 6H), 2.34 (s, 3H), 1.02 (t, J = 7.4 Hz, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ: 145.6, 142.2, 135.9, 135.7, 133.0, 128.2, 122.9, 115.7, 115.6, 85.1, 74.9, 53.4, 21.6, 8.9; HRMS (ESI) *m/z*: 467.1004, 469.0984 (Calcd for $C_{21}H_{28}BrN_2O_3S$ $[M]^+$: 467.1004, 469.0984).

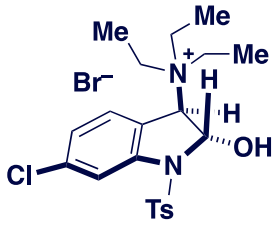
trans-2-Hydroxy-4-chloro-1-tosylindoline-3-ammonium bromide (3e)



To a solution of 4-chloro-1-tosylindole (612 mg, 2 mmol) and H_2O (0.36 mL, 20 mmol) in acetone (20 mL) was added NBS (392 mg, 2.2 mmol). The mixture was stirred at room temperature for 24 h. Then, Et_3N (0.31 mL, 2.2 mmol) was added to the mixture and stirred further 1 h. The mixture was concentrated *in vacuo*. and dried *in vacuo* to give **3e** (942 mg, 94% yield) without further purification.

942.0 mg, 94% yield. colorless oil; ^{1}H NMR (500 MHz, acetone-d_6) δ: 7.86 (d, J = 8.6 Hz, 2H), 7.42 (d, J = 8.0 Hz, 1H), 7.37 (t, J = 8.1 Hz, 1H), 7.36 (d, J = 8.1 Hz, 2H), 7.10 (d, J = 8.1 Hz, 1H), 6.05 (s, 1H), 5.13 (s, 1H), 2.58–2.60 (m, 6H), 2.35 (s, 3H), 1.03 (t, J = 6.9 Hz, 9H); ^{13}C NMR (125 MHz, acetone-d_6) δ: 144.9, 142.1, 136.1, 132.4, 131.8, 129.8, 128.1, 127.7, 124.3, 113.2, 93.5, 48.5, 46.1, 20.6, 10.7; HRMS (ESI) *m/z*: 423.1508, 425.1480 (Calcd for $C_{21}H_{28}ClN_2O_3S$ $[M]^+$: 423.1509, 425.1480).

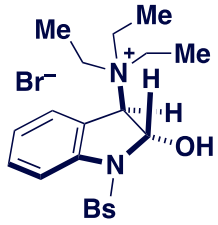
***trans*-2-Hydroxy-6-chloro-1-tosylindoline-3-ammonium bromide (3f)**



To a solution of 6-chloro-1-tosylindole (1.53 g, 5 mmol) and H_2O (0.90 mL, 50 mmol) in acetone (50 mL) was added NBS (979 mg, 5.5 mmol). The mixture was stirred at room temperature until the complete disappearance of starting material as indicated by TLC. Et_3N (0.77 mL, 5.5 mmol) was added to the mixture and stirred further 1 h. The resulting precipitate was separated by filtration, washed with acetone, and dried *in vacuo* to give **3f** (1.58 g, 63% yield).

1.58 g, 63% yield. colorless solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ: 8.04 (d, J = 8.6 Hz, 2H), 7.98 (d, J = 6.9 Hz, 1H), 7.56 (d, J = 8.6 Hz, 1H), 7.43 (d, J = 8.6 Hz, 2H), 7.29 (d, J = 2.3 Hz, 1H), 7.22 (dd, J = 2.3, 8.6 Hz, 1H), 6.39 (d, J = 6.3 Hz, 1H), 4.84 (s, 1H), 3.31–3.46 (m, 6H), 2.35 (s, 3H), 1.03 (t, J = 6.9 Hz, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ: 145.8, 144.1, 137.5, 135.8, 132.1, 130.7, 128.2, 124.0, 119.6, 113.3, 85.5, 74.8, 53.3, 21.6, 8.9; HRMS (ESI) *m/z*: 423.1511, 425.1480 (Calcd for $C_{21}H_{28}ClN_2O_3S$ $[M]^+$: 423.1509, 425.1480).

***trans*-2-Hydroxy-1-benzenesulfonylindoline-3-ammonium bromide (3g)**

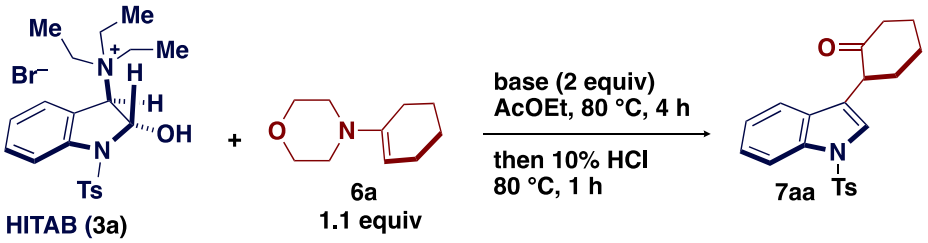


To a solution of 1-benzenesulfonylindole (5.15 g, 20 mmol) and H_2O (3.60 mL, 200 mmol) in acetone (200 mL) was added NBS (3.74 g, 21 mmol). The mixture was stirred at room temperature for 6 h. Et_3N (2.94 mL, 21 mmol) was added to the mixture and stirred further 1 h. The resulting precipitate was separated by filtration, washed with acetone, and dried *in vacuo* to give **3g** (7.47 g, 82% yield).

7.47 g, 82% yield. colorless solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ: 8.15 (d, J = 7.5 Hz, 2H), 7.90 (d, J = 6.9 Hz, 1H), 7.70 (t, J = 7.5 Hz, 1H), 7.61 (t, J = 7.4 Hz, 1H), 7.57 (d, J = 7.5 Hz, 1H), 7.49 (t, J = 8.0 Hz, 1H), 7.39 (d, J = 8.6 Hz, 1H), 7.15 (t, J = 8.1 Hz, 1H), 6.38 (d, J = 6.9 Hz, 1H), 4.85 (s, 1H), 3.33–3.47 (m, 6H), 1.01 (t, J = 6.9 Hz, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ: 142.7, 139.0, 134.7, 133.0, 130.5, 130.1, 128.1, 124.1, 120.5, 113.8, 84.8, 75.4, 53.3, 8.8; HRMS (ESI) *m/z*: 375.1742 (Calcd for $C_{20}H_{27}N_2O_3S$ $[M]^+$: 375.1742).

Optimization of Reaction Conditions

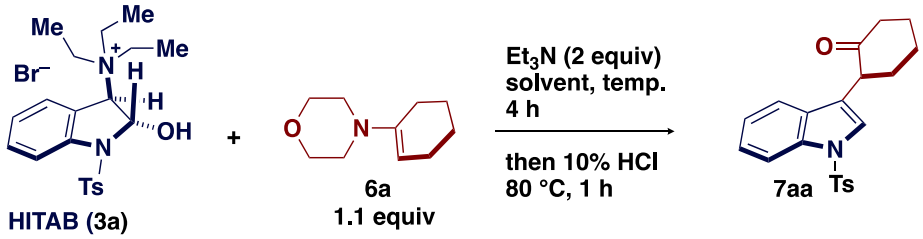
Table S1. Screening of bases



entry	base	% yield
1	Et_3N	86
2	TMEDA	43
3	iPr_2NEt	65
4	pyridine	67
5	DMAP	13
6	DABCO	46
7	DBU	8
8	K_2CO_3	0
9	Cs_2CO_3	0
10	NaOH	0
11	KOH	0

A mixture of **3a** (469.4 mg, 1.0 mmol), **6a** (183.5 mg, 1.1 mmol) and base (2.0 mmol) in AcOEt (10 mL) was heated at 80 °C with stirring for 4 h. After cooling to room temperature, 10% aq. HCl (10 mL) was added to the mixture. Then the mixture was heated at 80 °C for 1 h. After cooling to 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 = 1:5–1:2 or $CHCl_3$:hexane = 1:1) to give **7aa**.

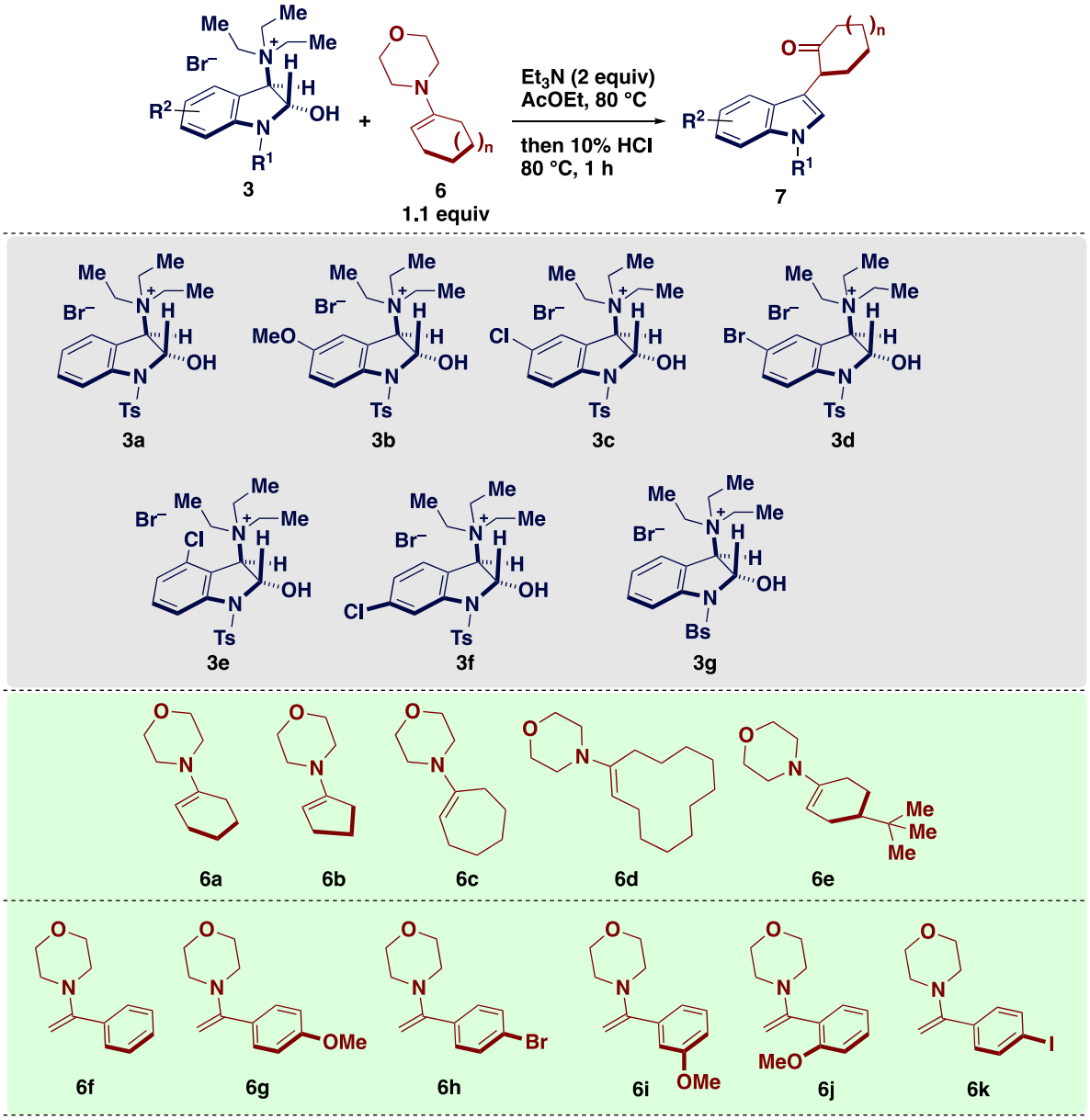
Table S2. Screening of solvents



entry	solvent	temp.	% yield
1	AcOEt	80	86
2	AcOEt	50	47
3	AcOEt	rt	4
4	benzene	80	80
5	toluene	80	83
6	hexane	80	64
7	1,4-dioxane	80	0
8	THF	80	0
9	MeCN	80	52
10	DMSO	80	0
11	DMF	80	13
12	$CHCl_3$	80	24

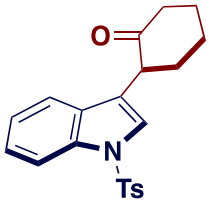
A mixture of **3a** (469.4 mg, 1.0 mmol), **6a** (183.5 mg, 1.1 mmol) and Et_3N (0.28 mL, 2.0 mmol) in solvent (10 mL) was heated at indicated temperature with stirring for 4 h. After cooling to room temperature, 10% aq. HCl (10 mL) was added to the mixture. Then the mixture was heated at 80 °C for 1 h. After cooling to 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 = 1:5–1:2 or $CHCl_3$:hexane = 1:1) to give **7aa**.

General Procedure for Synthesis of α-Indolylketones (Scheme 3)



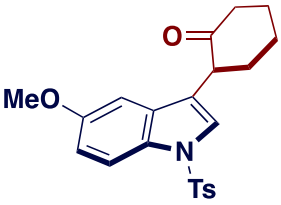
A mixture of **3** (1.0 mmol), **6** (1.1 mmol) and Et_3N (0.28 mL, 2.0 mmol) in AcOEt (10 mL) was heated at 80 °C with stirring for 2–16 h. After cooling to room temperature, 10% aq. HCl (10 mL) was added to the mixture. Then the mixture was heated at 80 °C for 1 h. After cooling to room temperature, 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 = 1:5–1:2 or $CHCl_3$:hexane = 1:1) to give **7**.

2-(1-Tosyl-1*H*-indol-3-yl)cyclohexan-1-one (7aa)



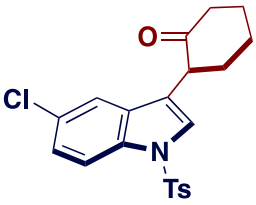
315.3 mg, 86% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.51 (s, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.28 (t, *J* = 8.6 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.19 (t, *J* = 8.0 Hz, 1H), 3.79 (dd, *J* = 11.5, 5.2 Hz, 1H), 2.45–2.55 (m, 2H), 2.33–2.39 (m, 1H), 2.32 (s, 3H), 2.12–2.19 (m, 1H), 2.00–2.08 (m, 2H), 1.80–1.90 (m, 2H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.1, 144.9, 135.4, 135.1, 130.5, 130.0, 126.9, 124.7, 123.8, 123.1, 120.5, 120.0, 113.8, 48.5, 42.1, 34.3, 28.1, 25.3, 21.6; HRMS (ESI) *m/z*: 390.1139 (Calcd for $C_{21}H_{21}NNaO_3S$ $[M+Na]^+$: 390.1140).

2-(5-Methoxy-1-tosyl-1*H*-indol-3-yl)cyclohexan-1-one (7ba)



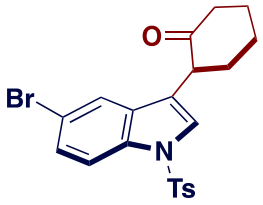
306.9 mg, 77% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.83 (d, *J* = 9.2 Hz, 1H), 7.71 (d, *J* = 8.6 Hz, 2H), 7.46 (s, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 6.88 (dd, *J* = 9.2, 2.3 Hz, 1H), 6.72 (d, *J* = 2.9Hz, 1H), 3.78 (s, 3H), 3.73 (dd, *J* = 11.4, 5.7 Hz, 1H), 2.44–2.54 (m, 2H), 2.32–2.37 (m, 1H), 2.32 (s, 3H), 2.11–2.19 (m, 1H), 2.00–2.08 (m, 2H), 1.81–1.90 (m, 2H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.0, 156.3, 144.8, 135.3, 131.6, 129.9, 126.8, 124.6, 120.6, 114.6, 113.4, 102.8, 55.8, 48.4, 42.0, 34.1, 28.0, 25.2, 21.6; HRMS (ESI) *m/z*: 420.1246 (Calcd for $C_{22}H_{23}NNaO_4S$ $[M+Na]^+$: 420.1246).

2-(5-Chloro-1-tosyl-1*H*-indol-3-yl)cyclohexan-1-one (7ca)



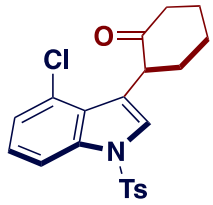
340.4 mg, 85% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.86 (d, *J* = 8.6 Hz, 1H), 7.72 (d, *J* = 8.6 Hz, 2H), 7.51 (s, 1H), 7.26 (d, *J* = 1.7 Hz, 1H), 7.21–7.23 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 3.73 (dd, *J* = 12.1, 5.2 Hz, 1H), 2.45–2.54 (m, 2H), 2.29–2.41 (m, 1H), 2.33 (s, 3H), 2.16–2.20 (m, 1H), 1.95–2.03 (m, 2H), 1.79–1.88 (m, 2H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 208.7, 145.2, 135.1, 133.5, 131.8, 130.1, 129.0, 126.9, 125.1, 124.9, 120.0, 119.8, 114.8, 48.3, 42.2, 34.3, 28.0, 25.4, 21.7; HRMS (ESI) *m/z*: 424.0750, 426.0721 (Calcd for $C_{21}H_{20}ClNNaO_3S$ $[M+Na]^+$: 424.0750, 426.0721).

2-(5-Bromo-1-tosyl-1*H*-indol-3-yl)cyclohexan-1-one (7da)



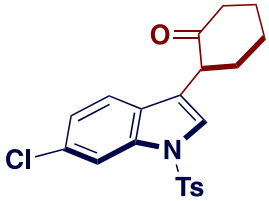
325.0 mg, 73% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.82 (d, *J* = 8.6 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.50 (s, 1H), 7.42 (s, 1H), 7.36 (d, *J* = 9.2 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 3.73 (dd, *J* = 11.5, 4.6 Hz, 1H), 2.46–2.55 (m, 2H), 2.33–2.36 (m, 1H), 2.33 (s, 3H), 2.17 (m, 1H), 1.95–2.04 (m, 2H), 1.84–1.88 (m, 2H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 208.6, 145.3, 135.1, 133.9, 132.3, 130.1, 127.6, 126.9, 125.0, 122.8, 119.9, 116.7, 115.2, 48.3, 42.2, 34.4, 28.0, 25.4, 21.7; HRMS (ESI) *m/z*: 468.0245, 470.0224 (Calcd for $C_{21}H_{20}BrNNaO_3S$ $[M+Na]^+$: 468.0245, 470.0224).

2-(4-Chloro-1-tosyl-1*H*-indol-3-yl)cyclohexan-1-one (7ea)



225.1 mg, 56% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.87 (d, *J* = 7.5 Hz, 1H), 7.73(d, *J* = 8.6 Hz, 2H), 7.50 (s, 1H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 7.5 Hz, 1H), 7.14 (d, *J* = 1.2 Hz, 1H), 4.41 (d, *J* = 11.5 Hz, 1H), 2.51–2.57 (m, 2H), 2.45–2.48 (m, 1H), 2.34 (s, 3H), 2.19–2.23 (m, 1H), 2.03–2.06 (m, 1H), 1.79–1.97 (m, 3H);^{13}C NMR (125 MHz, $CDCl_3$) δ:209.7, 145.3, 136.4, 135.0, 130.1, 127.5, 126.9, 126.5, 125.1, 124.8, 124.6, 120.5, 112.5, 49.2, 42.4, 34.5, 25.9, 21.7; HRMS (ESI) *m/z*: 424.0751, 426.0721 (Calcd for $C_{21}H_{20}ClNNaO_3S$ $[M+Na]^+$: 424.0750, 426.0721).

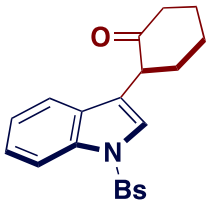
2-(6-Chloro-1-tosyl-1*H*-indol-3-yl)cyclohexan-1-one (7fa)



274.1 mg, 68% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (d, *J* = 1.7 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.47 (d, *J* = 1.1 Hz, 1H), 7.24 (d, *J* = 8.6 Hz, 2H), 7.21 (d, *J* = 6.9 Hz, 1H), 7.15 (dd, *J* = 8.6, 2.3 Hz, 1H), 3.75 (dd, *J* = 12.1, 5.8 Hz, 1H), 2.44–2.55 (m, 2H), 2.33–2.38 (m, 1H), 2.35 (s, 3H), 2.14–2.19 (m, 1H), 1.98–2.05 (m,

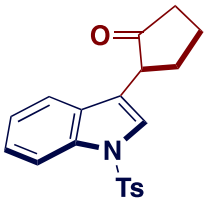
2H), 1.78–1.89 (m, 2H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 208.8, 145.3, 135.5, 135.1, 130.7, 130.1, 129.0, 126.9, 124.2, 123.8, 121.0, 120.4, 113.9, 48.3, 42.1, 34.2, 28.0, 25.3, 21.7; HRMS (ESI) *m/z*: 424.0750, 426.0721 (Calcd for $C_{21}H_{20}ClNNaO_3S$ $[M+Na]^+$: 424.0750, 426.0721).

2-(1-(Phenylsulfonyl)-1*H*-indol-3-yl)cyclohexan-1-one (7ga)



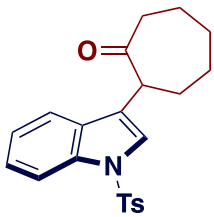
325.9 mg, 92% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 7.4 Hz, 2H), 7.51–7.53 (m, 2H), 7.43 (t, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 3.80 (dd, *J* = 11.5, 5.2 Hz, 1H), 2.46–2.56 (m, 2H), 2.33–2.41 (m, 1H), 2.14–2.20 (m, 1H), 2.00–2.08 (m, 2H), 1.81–1.90 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.0, 138.3, 135.2, 133.9, 130.5, 129.4, 126.8, 124.8, 123.7, 123.2, 120.8, 120.1, 113.8, 48.4, 42.1, 34.3, 28.1, 25.3; HRMS (ESI) *m/z*: 376.0983 (Calcd for $C_{20}H_{19}NNaO_3S$ $[M+Na]^+$: 376.0983).

2-(1-Tosyl-1*H*-indol-3-yl)cyclopentan-1-one (7ab)



229.0 mg, 65% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (d, *J* = 8.6 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.47 (d, *J* = 7.5 Hz, 1H), 7.43 (s, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 6.9 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 3.51 (t, *J* = 9.2 Hz, 1H), 2.45–2.55 (m, 2H), 2.27–2.38 (m, 1H), 2.31 (s, 3H), 2.13–2.19 (m, 1H), 2.05–2.10 (m, 1H), 1.97–2.02 (m, 1H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 216.9, 145.0, 135.3, 135.3, 130.3, 130.0, 126.9, 124.9, 123.2, 123.2, 120.4, 119.7, 113.7, 46.6, 38.1, 30.7, 21.6, 21.1; HRMS (ESI) *m/z*: 376.0984 (Calcd for $C_{20}H_{19}NNaO_3S$ $[M+Na]^+$: 376.0983).

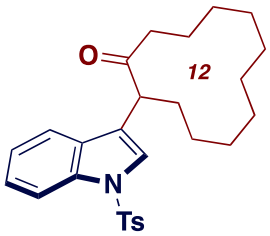
2-(1-Tosyl-1*H*-indol-3-yl)cycloheptan-1-one (7ac)



323.5 mg, 85% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.93 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.52 (s, 1H), 7.28 (td, *J* = 8.0, 1.2 Hz, 1H), 7.20–7.23 (m, 1H), 7.21 (d, *J* = 8.6 Hz,

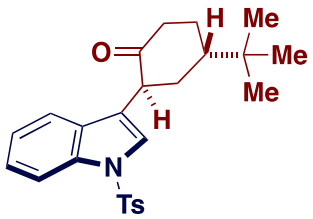
2H), 3.92 (dd, *J* = 11.5, 4.0 Hz, 1H), 2.68 (td, *J* = 13.2, 3.5 Hz, 1H), 2.42–2.47 (m, 1H), 2.33 (s, 3H), 2.19–2.24 (m, 1H), 1.89–2.06 (m, 4H), 1.61–1.69 (m, 1H), 1.43–1.52 (m, 2H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 211.9, 145.0, 135.3, 135.2, 130.2, 130.0, 126.9, 124.9, 123.5, 123.3, 121.6, 120.3, 113.7, 50.0, 41.6, 30.9, 29.9, 28.4, 25.4, 21.6; HRMS (ESI) *m/z*: 404.1296 (Calcd for $C_{22}H_{23}NNaO_3S$ $[M+Na]^+$: 404.1296).

2-(1-Tosyl-1*H*-indol-3-yl)cyclododecan-1-one (7ad)



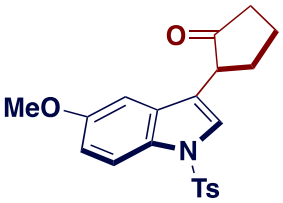
406.0 mg, 90% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.6 Hz, 2H), 7.51 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.30 (td, *J* = 6.9, 1.2 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 3.96 (dd, *J* = 12.0, 2.9 Hz, 1H), 2.52 (ddd, *J* = 17.2, 11.5, 2.9 Hz, 1H), 2.25–2.38 (m, 1H), 2.33 (s, 3H), 1.99–2.04 (m, 1H), 1.84–1.93 (m, 1H), 1.71–1.77 (m, 1H), 1.25–1.50 (m, 15H);^{13}C NMR (125 MHz, $CDCl_3$) δ:211.3, 145.1, 135.3, 135.2, 130.1, 130.0, 126.9, 125.1, 123.6, 123.5, 121.3, 119.7, 113.9, 49.0, 36.7, 29.4, 25.7, 25.4, 24.2, 24.1, 23.9, 23.5, 22.4, 22.3, 21.7; HRMS (ESI) *m/z*: 474.2080 (Calcd for $C_{27}H_{33}NNaO_3S$ $[M+Na]^+$: 474.2079).

***Rel*-(2*S*,4*S*)-4-(*tert*-butyl)-2-(1-tosyl-1*H*-indol-3-yl)cyclohexan-1-one (7ae)**



295.7 mg, 70% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 8.1 Hz, 1H), 7.77 (d, *J* = 8.6 Hz, 2H), 7.52 (s, 1H), 7.29 (d, *J* = 7.4 Hz, 1H), 7.26 (d, *J* = 5.2 Hz, 1H), 7.20 (d, *J* = 8.6 Hz, 2H), 7.17–7.22 (m, 1H), 3.82 (dd, *J* = 12.1, 5.2 Hz, 1H), 2.53–2.58 (m, 2H), 2.35–2.41 (m, 1H), 2.32 (s, 3H), 2.18–2.25 (m, 1H), 1.74–1.82 (m, 2H), 1.57–1.67 (m, 1H), 0.96 (s, 9H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.2, 144.9, 135.5, 135.1, 130.5, 130.0, 126.9, 124.6, 123.9, 123.1, 120.6, 119.9, 113.8, 47.8, 47.6, 41.7, 35.8, 32.7, 31.6, 28.8, 27.8, 27.6, 21.6; HRMS (ESI) *m/z*: 446.1766 (Calcd for $C_{25}H_{29}NNaO_3S$ $[M+Na]^+$: 446.1766).

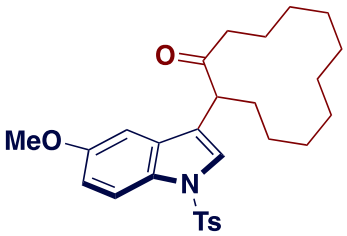
2-(5-Methoxy-1-tosyl-1*H*-indol-3-yl)cyclopentan-1-one (7bb)



236.6 mg, 62% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.83 (d, *J* = 9.8 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 2H),

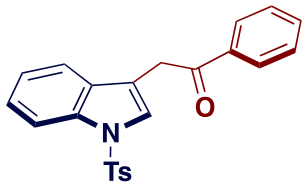
7.37 (s, 1H), 7.20 (d, J = 8.6 Hz, 2H), 6.90–6.92 (m, 2H), 3.80 (s, 3H), 3.46 (dd, J = 9.2, 8.0 Hz, 1H), 2.44–2.57 (m, 2H), 2.30–2.38 (m, 1H), 2.33 (s, 3H), 2.14–2.20 (m, 1H), 2.04–2.13 (m, 1H), 1.95–2.03 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 216.8, 156.4, 145.0, 135.2, 131.5, 130.0, 129.9, 126.8, 123.9, 119.9, 114.6, 113.7, 55.8, 46.6, 38.1, 30.5, 21.6, 21.1; HRMS (ESI) *m/z*: 406.1090 (Calcd for $C_{21}H_{21}NNaO_4S$ $[M+Na]^+$: 406.1089).

2-(5-Methoxy-1-tosyl-1*H*-indol-3-yl)cyclododecan-1-one (7bd)



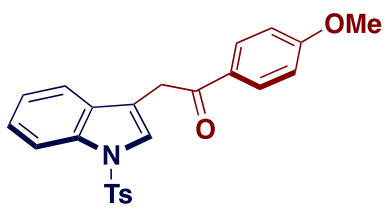
380.0 mg, 79% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.84 (d, J = 9.2 Hz, 1H), 7.70 (d, J = 8.6 Hz, 2H), 7.47 (s, 1H), 7.19 (d, J = 8.9 Hz, 2H), 6.90 (dd, J = 9.2, 2.3 Hz, 1H), 6.86 (d, J = 2.3 Hz, 1H), 3.87 (dd, J = 12.0, 2.9 Hz, 1H), 3.79 (s, 3H), 2.52 (ddd, J = 16.6, 11.5, 2.9 Hz, 1H), 2.32 (s, 3H), 2.24–2.32 (m, 1H), 1.85–1.97 (m, 2H), 1.24–1.50 (m, 16H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 211.2, 156.7, 145.0, 135.1, 131.1, 130.0, 129.9, 126.8, 124.4, 121.4, 114.8, 114.1, 102.1, 55.7, 49.4, 36.2, 29.2, 25.8, 25.5, 24.1, 24.0, 23.8, 23.5, 22.4, 22.2, 21.6; HRMS (ESI) *m/z*: 504.2185 (Calcd for $C_{28}H_{35}NNaO_4S$ $[M+Na]^+$: 504.2185).

1-phenyl-2-(1-tosyl-1*H*-indol-3-yl)ethan-1-one (7af)



315.5 mg, 81% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.01 (d, J = 6.9 Hz, 2H), 7.96 (d, J = 8.6 Hz, 1H), 7.70 (d, J = 8.6 Hz, 2H), 7.58 (t, J = 7.5 Hz, 1H), 7.54 (s, 1H), 7.45–7.49 (m, 3H), 7.31 (t, J = 7.4 Hz, 1H), 7.23 (t, J = 6.9 Hz, 1H), 7.16 (d, J = 8.0 Hz, 2H), 4.32 (s, 2H), 2.31 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 196.3, 144.9, 136.3, 135.3, 135.2, 133.5, 130.8, 129.9, 128.8, 128.6, 126.9, 125.1, 125.0, 123.4, 119.7, 115.9, 113.8, 35.3, 21.6; HRMS (ESI) *m/z*: 412.0984 (Calcd for $C_{23}H_{19}NNaO_3S$ $[M+Na]^+$: 412.0983).

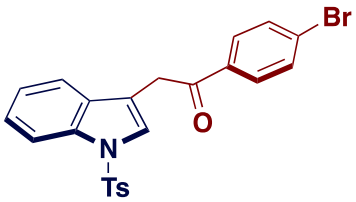
1-(4-Methoxyphenyl)-2-(1-tosyl-1*H*-indol-3-yl)ethan-1-one (7ag)



328.1 mg, 78% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.98 (d, J = 9.2 Hz, 2H), 7.96 (d, J = 8.6 Hz, H), 7.69 (d, J = 8.6 Hz, 2H), 7.51 (s, 1H), 7.48 (d, J = 8.1 Hz, 1H), 7.30 (t, J = 7.5 Hz, 1H), 7.22 (t, J = 8.1 Hz, 1H), 7.15 (d, J = 8.0 Hz, 2H), 6.92 (d, J = 9.2 Hz, 2H), 4.26 (s, 2H), 3.86 (s, 3H), 2.30 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$) δ:

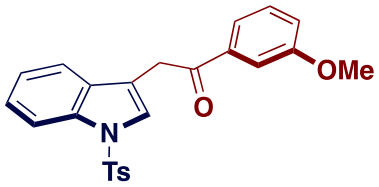
195.0, 163.8, 144.9, 135.3, 135.2, 130.9, 130.8, 129.9, 129.4, 126.9, 124.9, 123.4, 119.7, 116.4, 114.0, 113.8, 55.6, 35.0, 21.6; HRMS (ESI) *m/z*: 442.1088 (Calcd for $C_{24}H_{21}NNaO_4S$ $[M+Na]^+$: 442.1089).

1-(4-Bromophenyl)-2-(1-tosyl-1*H*-indol-3-yl)ethan-1-one (7ah)



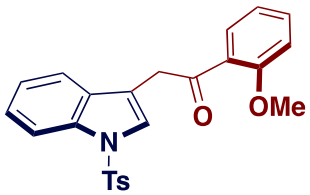
352.2 mg, 75% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (d, *J* = 8.6 Hz, 1H), 7.84 (d, *J* = 8.6 Hz, 2H), 7.68 (d, *J* = 8.6 Hz, 2H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.51 (s, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 8.1 Hz, 1H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.16 (d, *J* = 8.6 Hz, 2H), 4.27 (s, 2H), 2.32 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$) δ:195.4, 145.0, 135.2, 135.1, 132.1, 130.6, 130.1, 129.9, 128.7, 126.8, 125.1, 125.0, 123.5, 119.6, 115.6, 113.9, 35.4, 21.7; HRMS (ESI) *m/z*: 490.0089, 492.0067 (Calcd for $C_{23}H_{18}BrNNaO_3S$ $[M+Na]^+$: 490.0088, 492.0068).

1-(3-Methoxyphenyl)-2-(1-tosyl-1*H*-indol-3-yl)ethan-1-one (7ai)



184.6 mg, 44% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (d, *J* = 8.1 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.59 (dd, *J* = 8.6, 1.2 Hz, 1H), 7.53 (s, 1H), 7.51 (dd, *J* = 2.9, 1.7 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 8.6 Hz, 1H), 7.31 (td, *J* = 7.5, 1.2 Hz, 1H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.12 (dd, *J* = 8.0, 3.4 Hz, 1H), 4.30 (s, 2H), 3.82 (s, 3H), 2.32 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 196.2, 160.0, 144.9, 137.7, 135.3, 135.2, 130.8, 129.9, 129.8, 126.9, 125.1, 125.0, 123.4, 121.2, 120.0, 119.6, 115.9, 113.8, 112.7, 55.5, 35.4, 21.6; HRMS (ESI) *m/z*: 442.1089 (Calcd for $C_{24}H_{21}NNaO_4S$ $[M+Na]^+$: 442.1089).

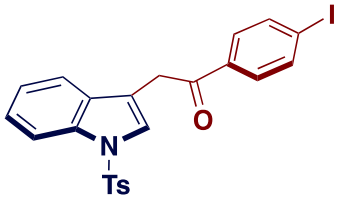
1-(2-Methoxyphenyl)-2-(1-tosyl-1*H*-indol-3-yl)ethan-1-one (7aj)



288.2 mg, 69% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.94 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.6 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.49 (s, 1H), 7.45 (d, *J* = 8.6 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.21 (t, *J* = 6.9 Hz, 1H), 7.15 (d, *J* = 8.6 Hz, 2H), 6.98 (t, *J* = 7.5 Hz, 1H), 6.95 (d, *J* = 8.6 Hz, 1H), 4.34 (s, 2H), 3.86 (s, 3H), 2.30 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 198.7, 158.5, 144.8, 135.4, 135.1, 133.9, 131.2, 130.8, 129.9, 127.7, 126.8, 124.8, 124.7, 123.3, 120.9, 119.8, 116.6, 113.7, 111.6, 55.6, 40.0, 21.6; HRMS (ESI) *m/z*: 442.1089 (Calcd for $C_{24}H_{21}NNaO_4S$

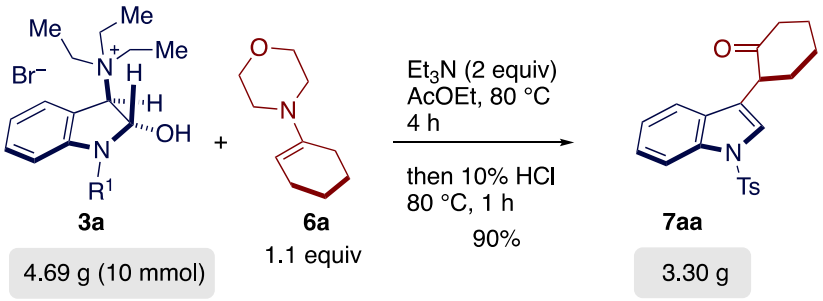
[M+Na]$^+$: 442.1089).

1-(4-Iodophenyl)-2-(1-tosyl-1*H*-indol-3-yl)ethan-1-one (7ak)



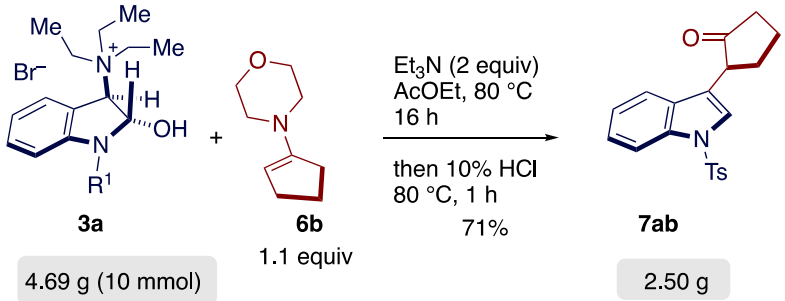
313.3 mg, 61% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (d, J = 8.6 Hz, 1H), 7.80 (d, J = 8.6 Hz, 2H), 7.69 (d, J = 1.7 Hz, 2H), 7.67 (d, J = 1.7 Hz, 2H), 7.51 (s, 1H), 7.45 (d, J = 8.0 Hz, 1H), 7.31 (t, J = 7.5 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 7.16 (d, J = 8.0 Hz, 2H), 4.26 (s, 2H), 2.32 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 195.7, 145.0, 138.1, 138.0, 135.5, 135.2, 135.1, 130.6, 129.9, 126.8, 125.1, 125.0, 123.5, 119.6, 115.6, 113.9, 101.5, 35.3, 21.7; HRMS (ESI) *m/z*: 537.9950 (Calcd for $C_{23}H_{18}INNaO_3S$ [M+Na]$^+$: 537.9950).

Procedure for Gram-Scale Synthesis of 7aa (Scheme 4)



A mixture of **3a** (4.69 g, 10 mmol), **6a** (1.84 g, 11 mmol) and Et_3N (2.8 mL, 20 mmol) in AcOEt (100 mL) was heated at 80 °C with stirring for 4 h. After cooling to room temperature, 10% aq. HCl (50 mL) was added to the mixture. Then the mixture was heated at 80 °C for 1 h. After cooling to room temperature, the whole was extracted with AcOEt (3 x 100 mL), washed with brine (50 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 then $CHCl_3$:hexane = 1:1) to give **7aa** (3.30 g, 90%).

Procedure for Gram-Scale Synthesis of 7ab (Scheme 4)



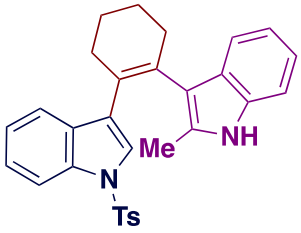
A mixture of **3a** (4.69 g, 10 mmol), **6b** (1.69 g, 11 mmol) and Et_3N (2.8 mL, 20 mmol) in AcOEt (100 mL) was

heated at 80 °C with stirring for 16 h. After cooling to room temperature, 10% aq. HCl (50 mL) was added to the mixture. Then the mixture was heated at 80 °C for 1 h. After cooling to room temperature, the whole was extracted with AcOEt (3 x 100 mL), washed with brine (50 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 then $CHCl_3$:hexane = 1:1) to give **7ab** (2.50 g, 71%).

General Procedure for Synthesis of Bisindoles using $In(OTf)_3$ (Scheme 5)

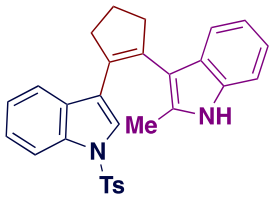
To a solution of **7aa** (367.5 mg, 1.0 mmol) or **7ab** (353.4 mg, 1.0 mmol) and 2-methylindole (262.2 mg, 2.0 mmol) or indole (234.1 mg, 2.0 mmol) in MeCN (10 mL) was added $In(OTf)_3$ (56.2 mg, 0.1 mmol) at room temperature and the mixture was stirred at 100 °C for 16 h. After cooling to room temperature, 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 ($CHCl_3$:hexane = 1:1) to give bisindoles.

2-Methyl-3-(2-(1-tosyl-1*H*-indol-3-yl)cyclohex-1-en-1-yl)-1*H*-indole (8)



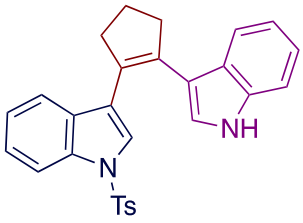
268.2 mg, 56% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.75 (d, *J* = 8.6 Hz, 1H), 7.48 (dd, *J* = 1.7, 6.9 Hz, 1H), 7.37 (br s, 1H), 7.33 (d, *J* = 8.6 Hz, 2H), 7.17 (d, *J* = 7.5 Hz, 2H), 7.13 (dd, *J* = 1.8, 5.8 Hz, 1H), 7.02–7.09 (m, 5H), 6.87 (t, *J* = 7.4 Hz, 1H), 2.72–2.76 (m, 1H), 2.56–2.65 (m, 1H), 2.37–2.50 (m, 1H), 2.31 (s, 3H), 2.20–2.33 (m, 1H), 1.86–1.98 (m, 4H), 1.79 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$) δ: 144.5, 135.3, 135.2, 134.7, 131.4, 130.7, 130.1, 129.8, 128.4, 128.1, 126.6, 126.2, 124.0, 123.5, 122.6, 121.1, 120.9, 119.5, 119.0, 115.9, 113.3, 110.2, 32.0, 31.9, 23.6, 23.4, 21.7, 12.4; HRMS (ESI) *m/z*: 503.1768 (Calcd for $C_{30}H_{28}N_2NaO_2S$ $[M+Na]^+$: 503.1769).

2-Methyl-3-(2-(1-tosyl-1*H*-indol-3-yl)cyclopent-1-en-1-yl)-1*H*-indole (9)



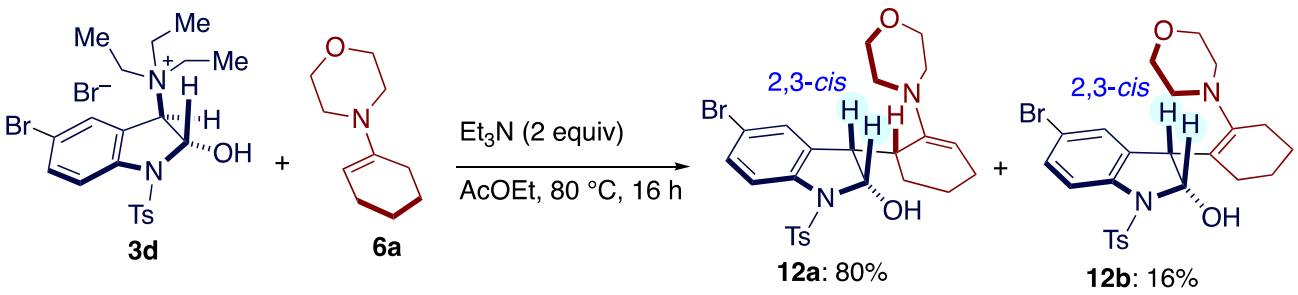
318.2 mg, 68% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.90 (d, *J* = 8.6 Hz, 1H), 7.64 (br s, 1H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.38 (s, 1H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.11–7.16 (m, 4H), 7.03 (t, *J* = 8.1 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 6.83 (t, *J* = 8.0 Hz, 1H), 3.06 (t, *J* = 7.5 Hz, 4H), 2.32 (s, 3H), 2.17 (quint, *J* = 7.4 Hz, 2H), 1.67 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 144.7, 135.6, 135.1, 135.0, 134.1, 132.1, 129.8, 129.6, 129.5, 127.9, 126.8, 124.2, 124.1, 122.8, 122.2, 121.9, 121.2, 119.7, 119.6, 113.5, 111.5, 110.4, 38.8, 38.0, 23.3, 21.6, 12.7; HRMS (ESI) *m/z*: 489.1612 (Calcd for $C_{29}H_{26}N_2NaO_2S$ $[M+Na]^+$: 489.1613).

3-(2-(1*H*-Indol-3-yl)cyclopent-1-en-1-yl)-1-tosyl-1*H*-indole (10)



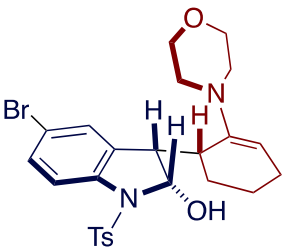
234.0 mg, 52% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.95 (br s, 1H), 7.88 (d, *J* = 8.6 Hz, 1H), 7.59 (d, *J* = 8.6 Hz, 2H), 7.40 (s, 1H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.16–7.17 (m, 3H), 7.07–7.10 (m, 2H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 2.3 Hz, 1H), 6.76 (t, *J* = 8.5 Hz, 1H), 3.04–3.08 (m, 2H), 2.93–2.95 (m, 2H), 2.35 (s, 3H), 2.14 (quint, *J* = 7.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 144.7, 136.0, 135.3, 135.0, 133.6, 129.9, 129.6, 127.1, 126.9, 125.9, 124.2, 123.6, 122.8, 122.1, 121.9, 121.7, 121.1, 119.7, 114.6, 113.4, 111.1, 39.0, 38.9, 22.8, 21.7; HRMS (ESI) *m/z*: 475.1457 (Calcd for $C_{28}H_{24}N_2NaO_2S$ $[M+Na]^+$: 475.1456).

General Procedure for Synthesis of Enamines (Scheme 6a)



A mixture of **3d** (548.3 mg, 1.0 mmol), **6a** (184 mg, 1.1 mmol) and Et_3N (0.28 mL, 2.0 mmol) in AcOEt (10 mL) was heated at 80 °C with stirring for 16 h. After cooling to room temperature, H_2O (10 mL) was added to the mixture. 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 = 1:5–1:2 then $CHCl_3$:hexane = 1:1) to give **12a** (425.2 mg, 80% yield) and **12b** (86.4 mg, 16% yield).

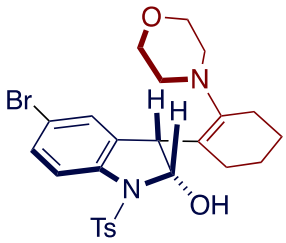
***Rel*-(2*S*,3*S*)-5-bromo-3-((*R*)-2-morpholinocyclohex-2-en-1-yl)-1-tosylindolin-2-ol (12a)**



425.2 mg, 80% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.82 (d, *J* = 8.6 Hz, 2H), 7.23–7.28 (m, 5H), 7.11 (s, 1H), 5.99 (d, *J* = 7.5 Hz, 1H), 4.14 (t, *J* = 8.0 Hz, 1H), 3.64–3.72 (m, 4H), 2.79–2.80 (m, 2H), 2.54–2.58 (m, 2H), 2.45 (dt, *J* = 7.4, 6.3 Hz, 1H), 2.38 (s, 3H), 1.40–1.52 (m, 2H), 1.10–1.17 (m, 2H), 0.94–1.00 (m, 1H), 0.40–

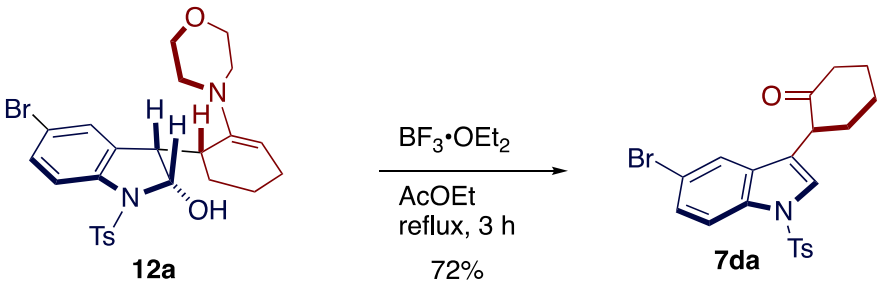
0.47 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 144.3, 141.6, 136.2, 132.1, 131.1, 129.7, 128.9, 127.6, 115.5, 114.8, 99.0, 94.8, 67.8, 49.8, 45.7, 40.7, 27.0, 24.3, 24.2, 21.7, 21.5; HRMS (ESI) *m/z*: 555.0929, 557.0908 (Calcd for $C_{25}H_{29}BrN_2NaO_4S$ $[M+Na]^+$: 555.0929, 557.0909).

***Rel*-(2*S*,3*S*)-5-bromo-3-(2-morpholinocyclohex-1-en-1-yl)-1-tosylindolin-2-ol (12b)**



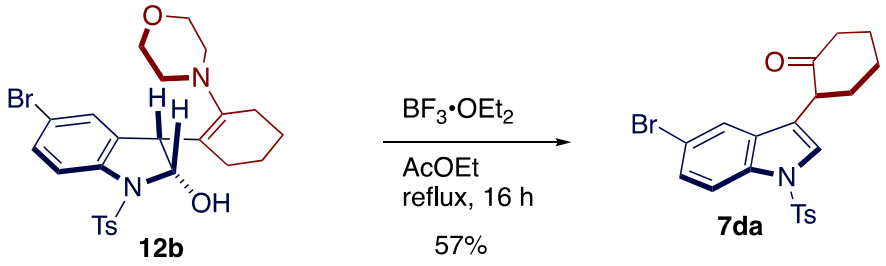
86.4 mg, 16% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.74 (d, *J* = 8.6 Hz, 2H), 7.34 (d, *J* = 9.2 Hz, 1H), 7.23–7.27 (m, 4H), 7.11 (s, 1H), 6.18 (d, *J* = 7.4 Hz, 1H), 3.32 (d, *J* = 6.9 Hz, 1H), 3.08 (m, 2H), 2.54 (m, 2H), 2.47 (dd, *J* = 11.5, 6.3 Hz, 1H), 2.37 (s, 3H), 2.12–2.16 (m, 2H), 1.89–1.96 (m, 2H), 1.58–1.64 (m, 3H), 1.32–1.42 (m, 2H), 1.05–1.08 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 144.3, 141.3, 136.8, 136.2, 130.2, 129.9, 127.1, 126.0, 115.6, 115.1, 98.9, 95.3, 66.5, 53.2, 45.9, 43.6, 31.9, 24.4, 23.8, 21.8, 21.6; HRMS (ESI) *m/z*: 555.0928, 557.0909 (Calcd for $C_{25}H_{29}BrN_2NaO_4S$ $[M+Na]^+$: 555.0929, 557.0909).

Conversion of 12a into 7da (Scheme 6b)



To a solution of **12a** (53.4 mg, 0.1 mmol) in AcOEt (2 mL) was added BF_3•Et_2O (0.06 mL, 0.5 mmol) and heated at 90 °C (oil bath) with stirring for 3 h. After cooling to room temperature, saturated aq. $NaHCO_3$ was added to the mixture. The whole was extracted with AcOEt (3 x 10 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 ($CHCl_3$:hexane = 1:1) to give **7da** (32.3 mg, 72% yield).

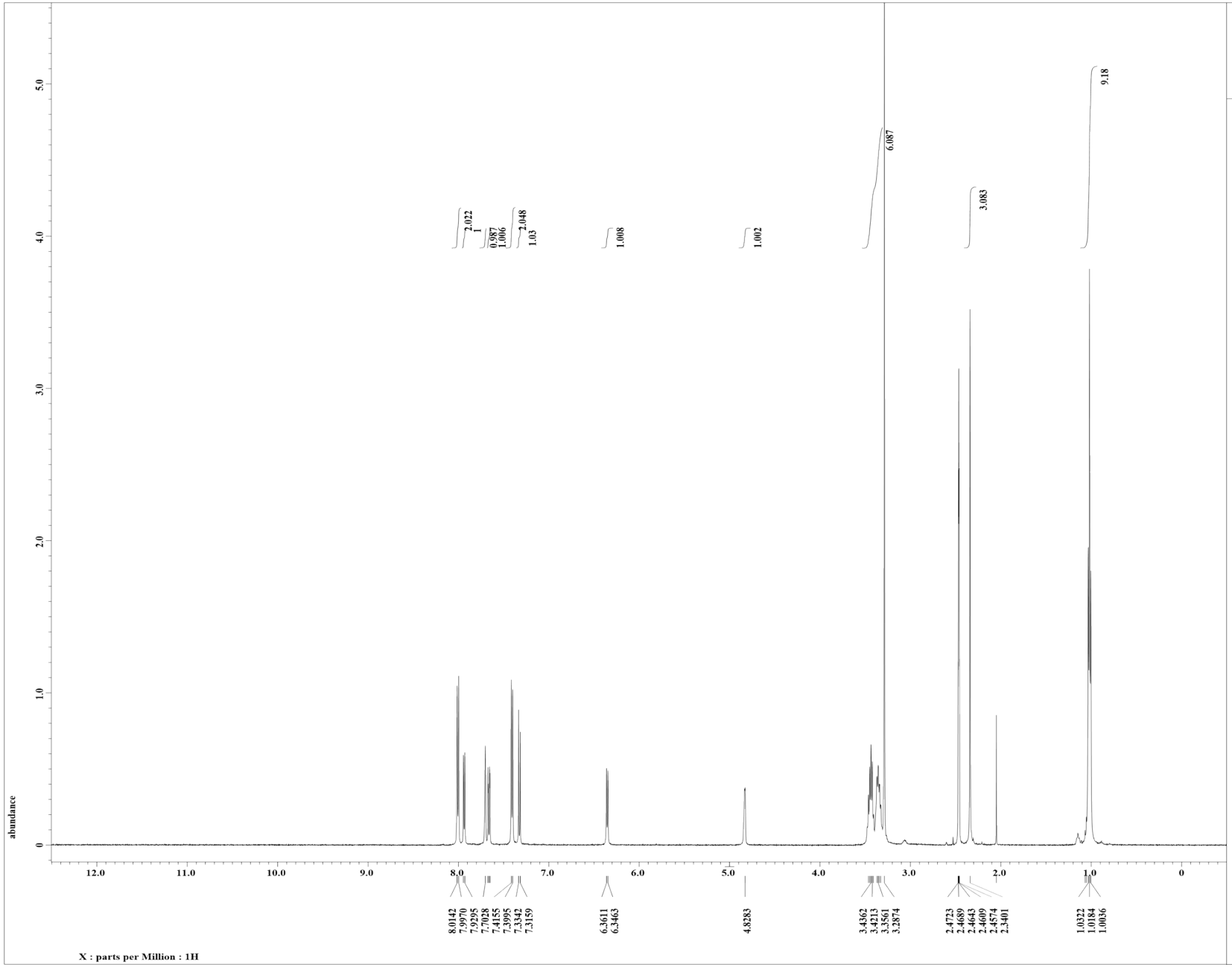
Conversion of 12b into 7da (Scheme 6c)



To a solution of **12a** (53.4 mg, 0.1 mmol) in AcOEt (2 mL) was added BF_3•Et_2O (0.06 mL, 0.5 mmol) and heated at 90 °C (oil bath) with stirring for 16 h. After cooling to room temperature, saturated aq. $NaHCO_3$ was added to the mixture. The whole was extracted with AcOEt (3 x 10 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 ($CHCl_3$:hexane = 1:1) to give **7da** (30.4 mg, 57% yield).

3. Supplementary References

(S1) Abe, T.; Kosaka, Y.; Kawasaki, T.; Ohata, Y.; Yamada, K. *Chem. Pharm Bull.,* **2020**, *68*; 555–558.
(S2) Abe, T.; Suzuki, T.; Anada, M.; Matsunaga, S.; Yamada, K.; *Org. Lett.,* **2017**, *19*, 4275–4278.
(S3) Hirao, S.; Yamashiro, T.; Kohira, K.; Mishima, N.; Abe, T. *Chem. Commun.* **2020**, *56,* 5139–5142.
(S4) Xing, D.; Dong, G. *J. Am. Chem. Soc*., **2017**, *139*, 13664–13667.



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X_sweep           = 9.28677563[kHz]
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Irr_offset        = 5[ppm]
Tri_domain        = 1H
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Tri_offset        = 5[ppm]
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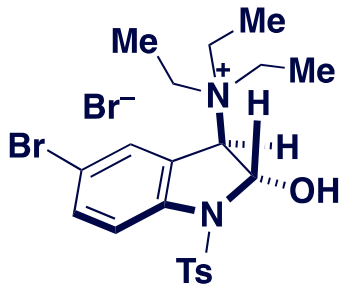

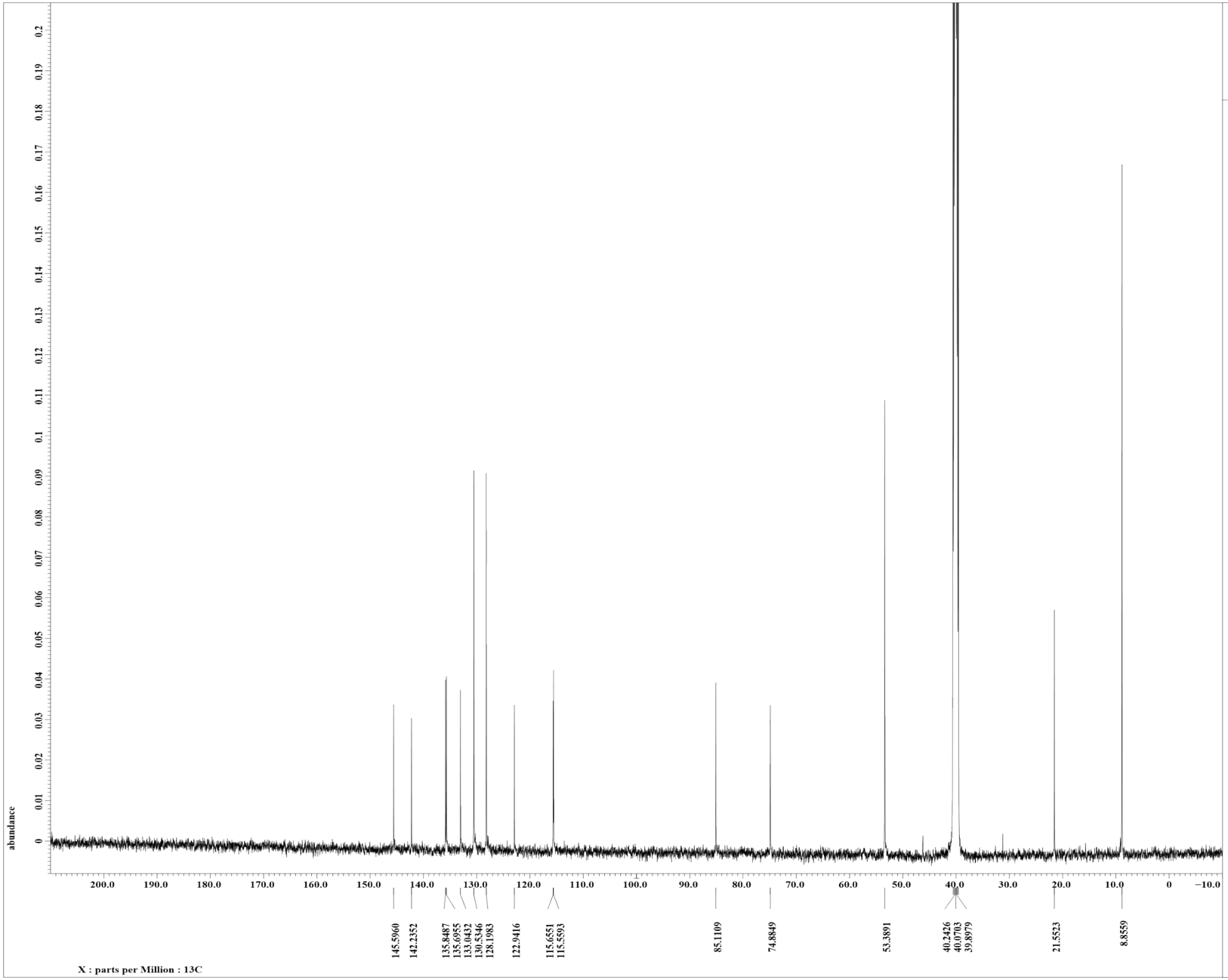


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Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
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Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 21840
Total_scans       = 21840

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
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Irr_atn_dec       = 21.51[dB]
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Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 24.9[dC]
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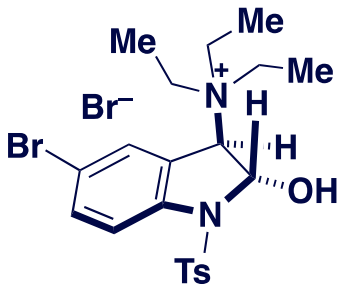

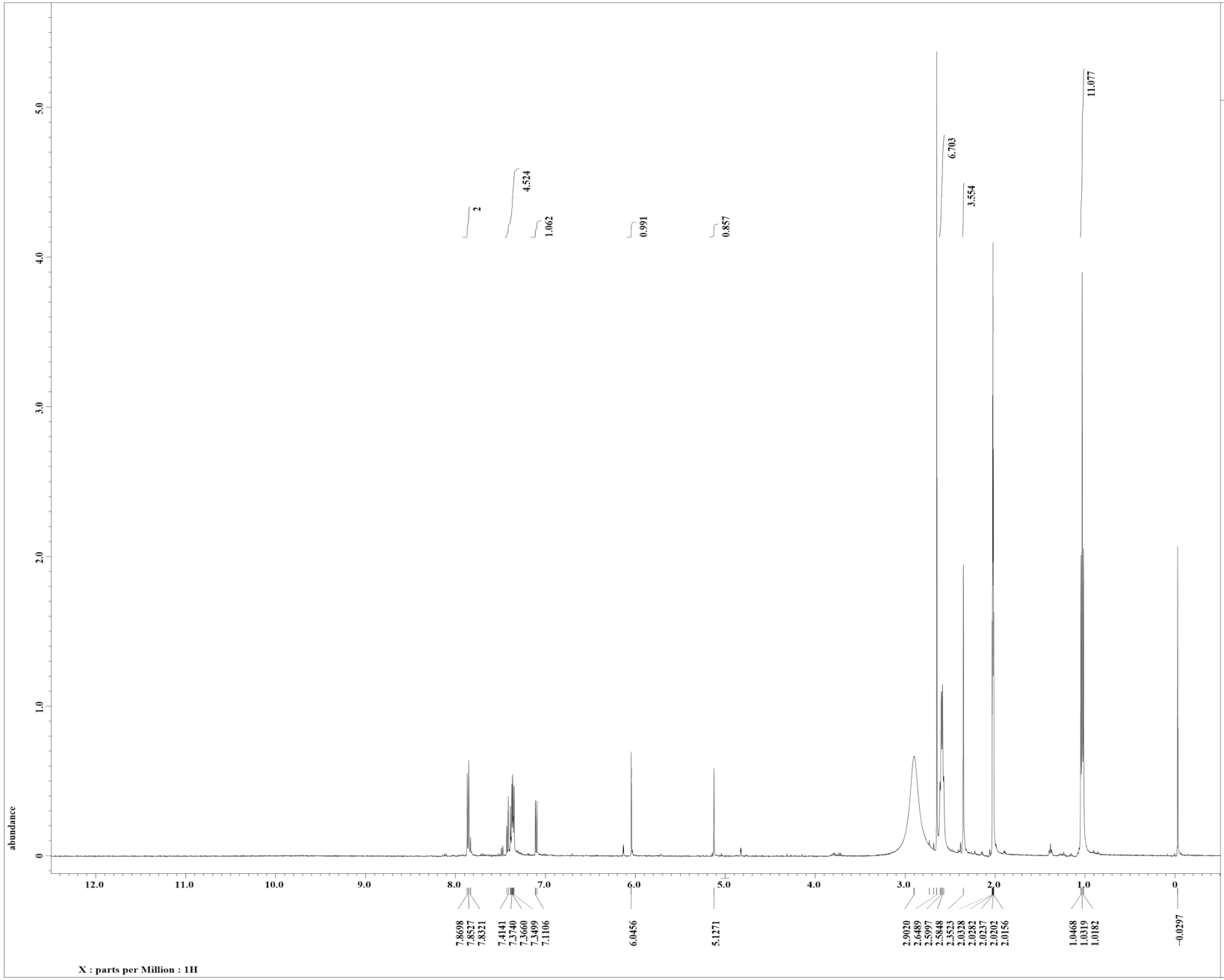


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Revision_time     =  8-JUL-2020 17:12:12
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Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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X_sweep           = 9.38438438[kHz]
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Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
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X_90_width        = 12[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
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Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
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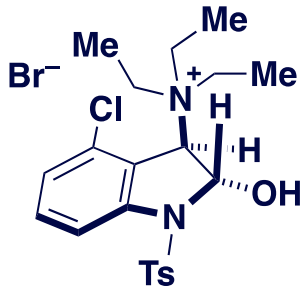

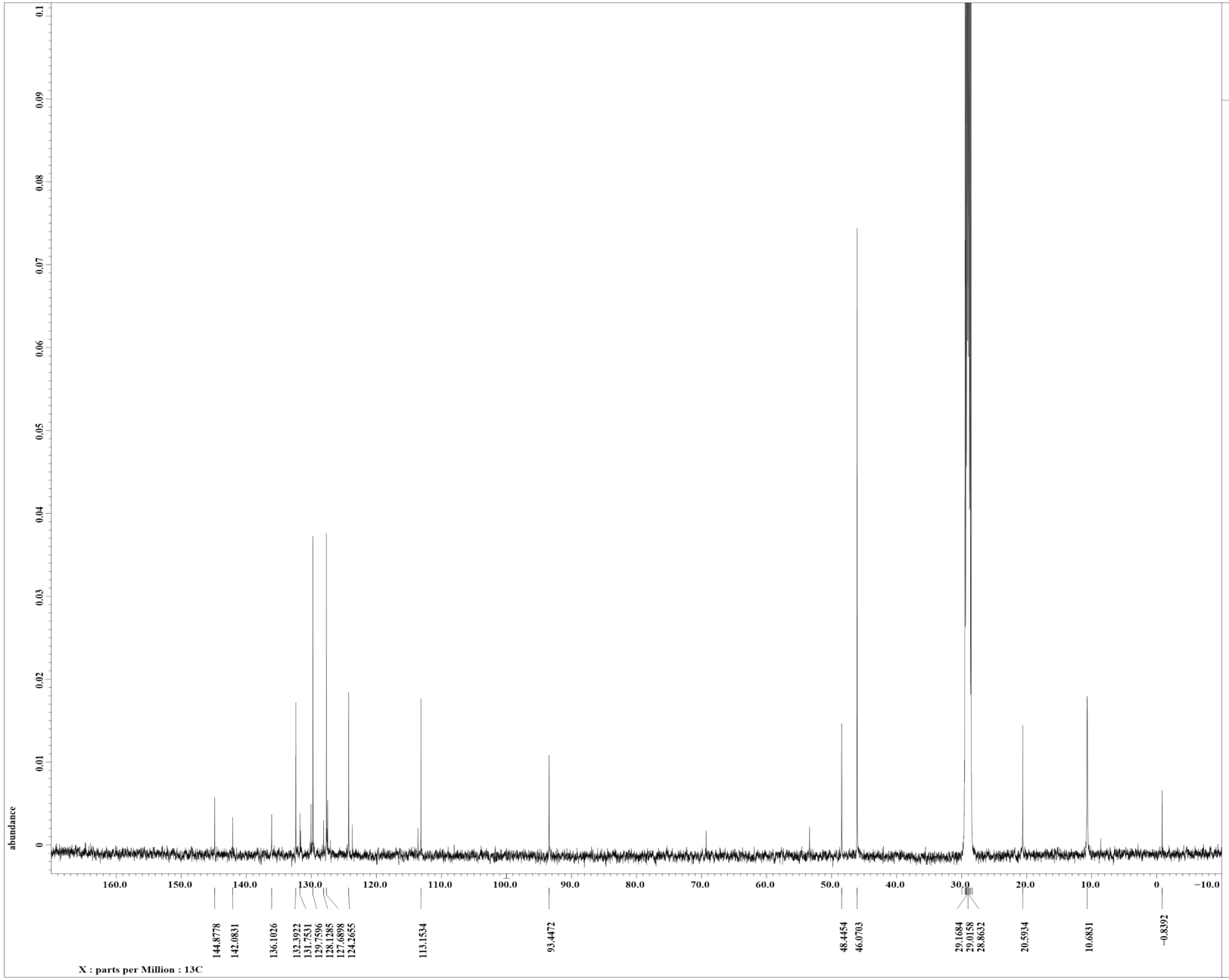
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0.02
0.01
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120.0
110.0
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90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
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142.0831
136.1026
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129.7596
128.1285
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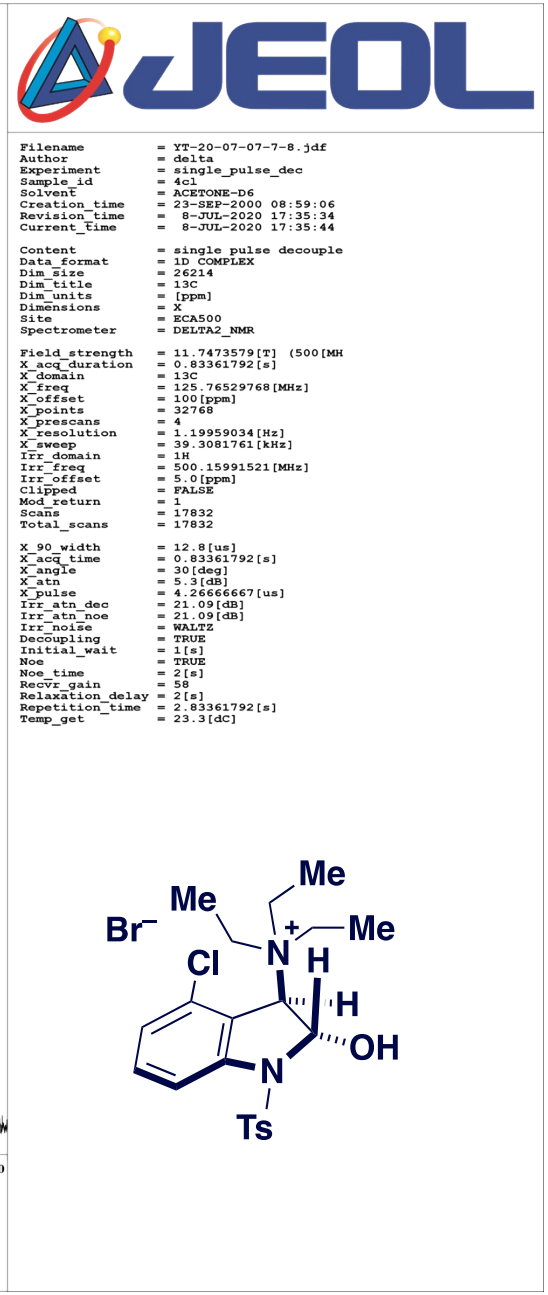
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Irr_noise = WALTZ
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Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 58
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
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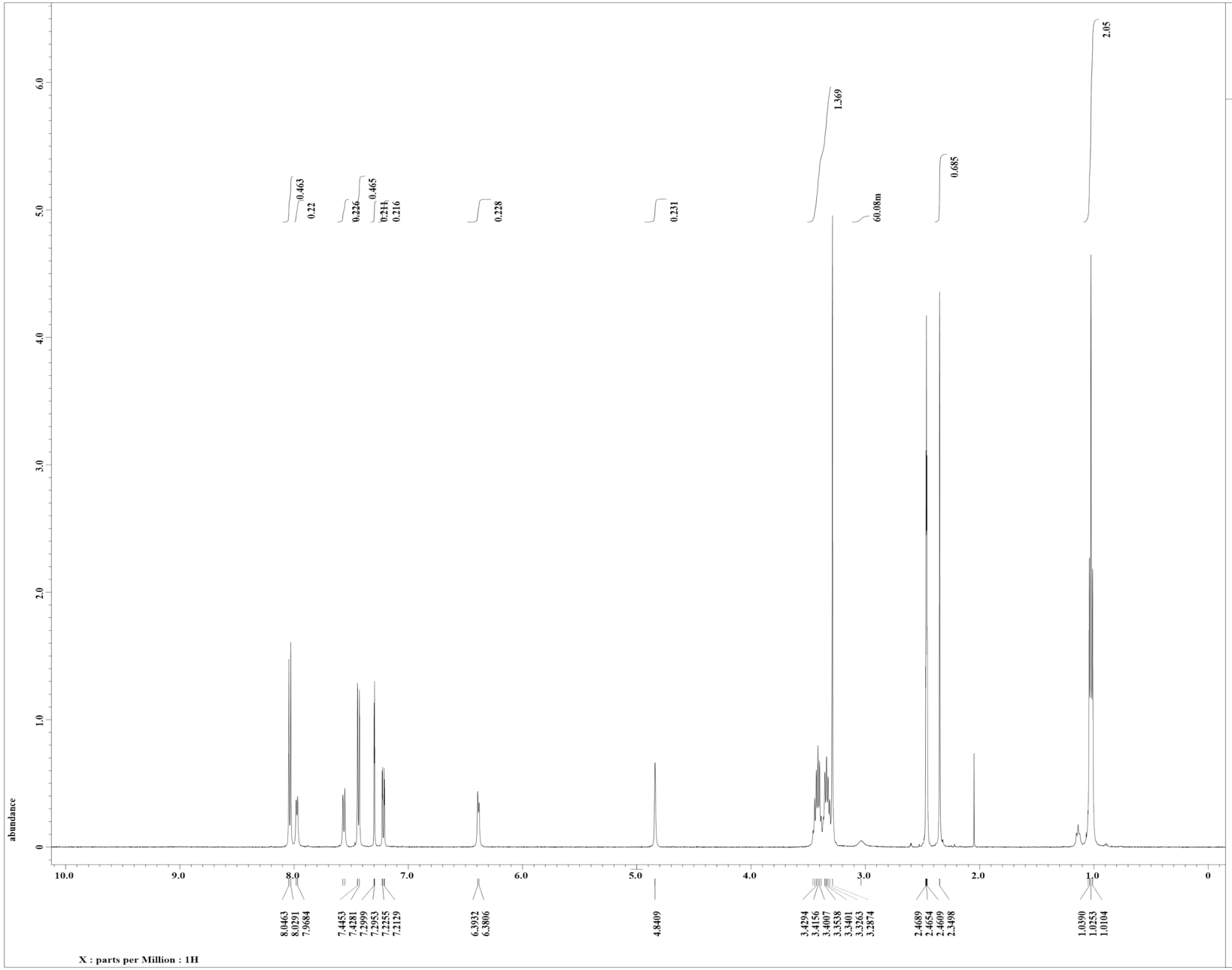
Cl
H
H
OH
N
Ts



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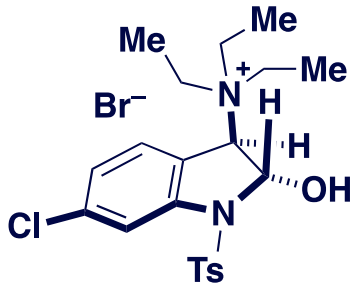
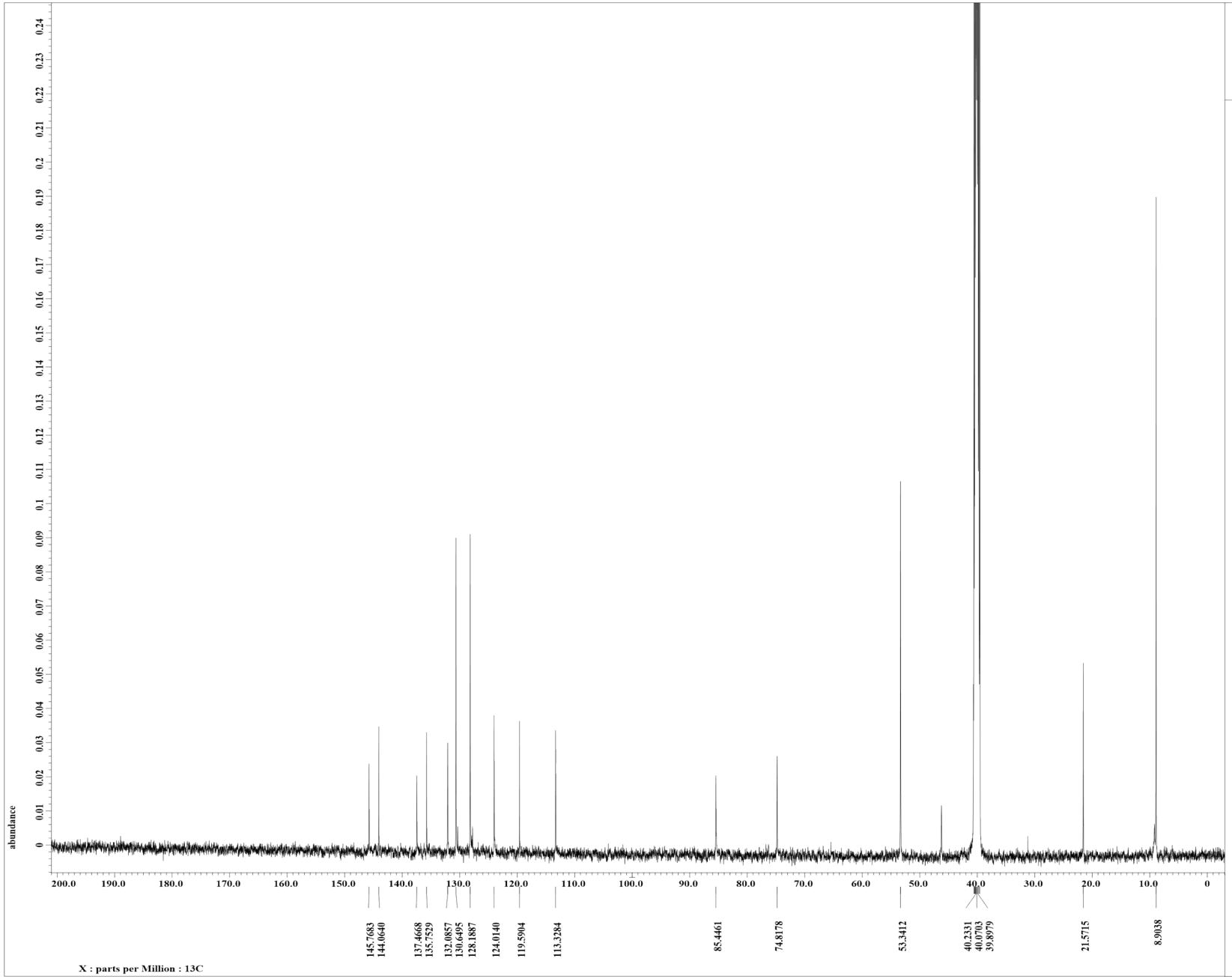
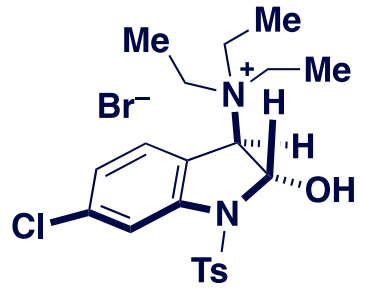
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

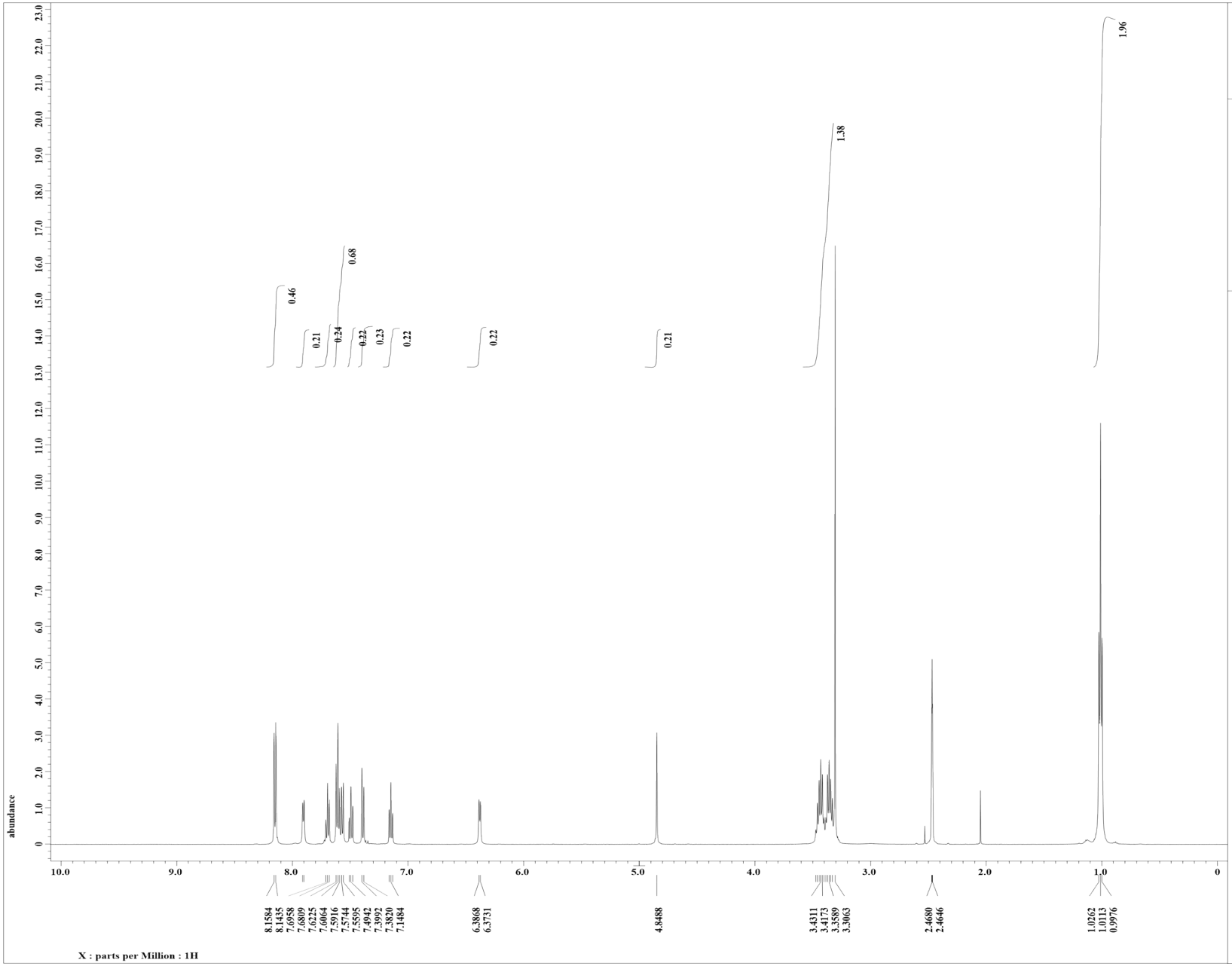
X_90_width = 11.3[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_pulse = 5.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 48
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 24.1[dC]





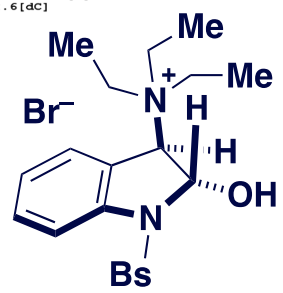
```
Filename          = 6Cl-HITAB-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#739786
Solvent           = DMSO-D6
Creation_time     = 10-JUN-2020 06:32:12
Revision_time     = 10-JUN-2020 07:14:28
Current_time      = 10-JUN-2020 07:15:21

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 13526
Total_scans       = 13526

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 25[dC]
```

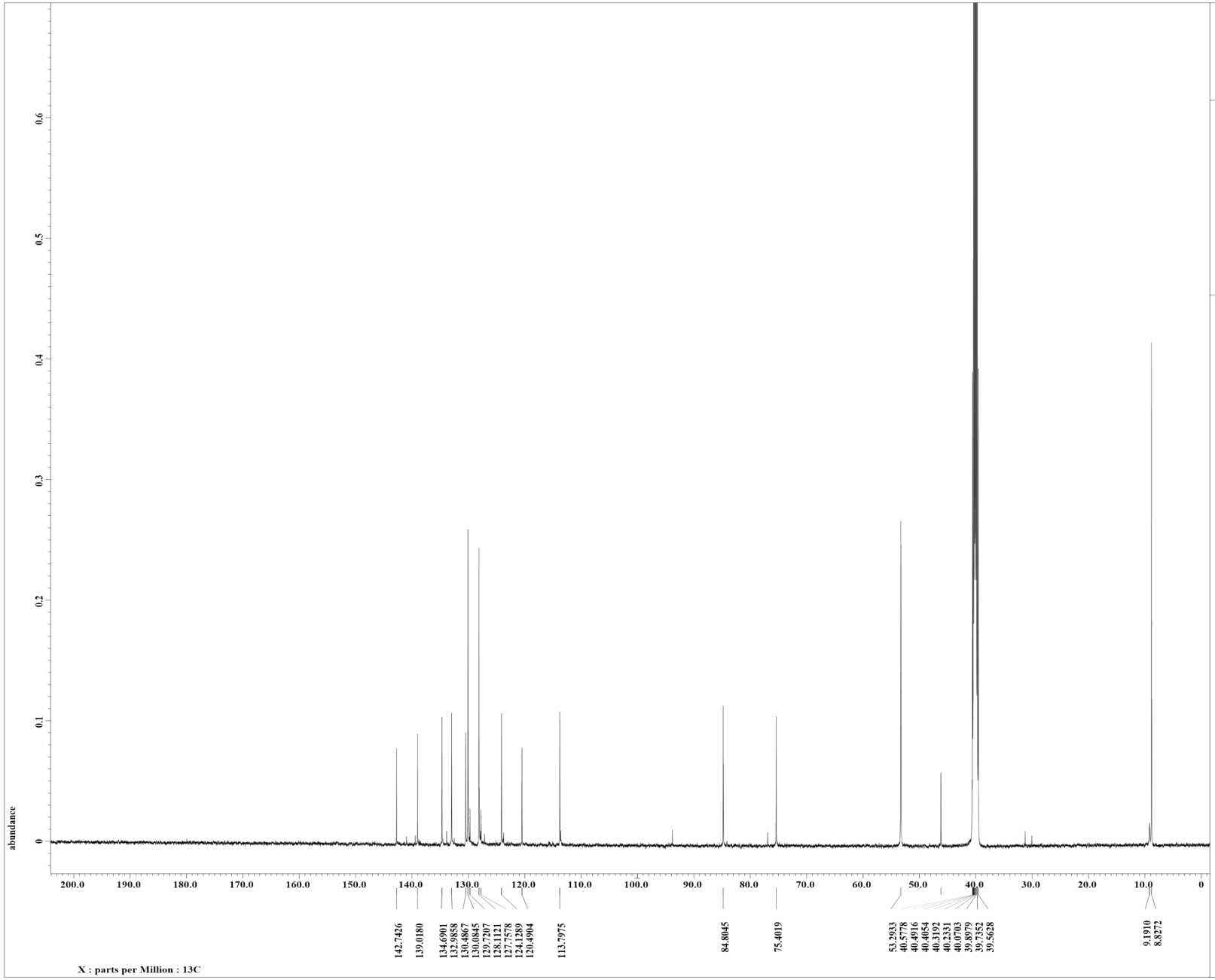





```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2020-0414-2.jdf
```

```
Filename          = TA2020-0414-5.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#378727
Solvent           = DMSO-D6
Creation_time     = 30-JUN-2000 12:17:14
Revision_time     = 14-APR-2020 10:34:41
Current_time      = 14-APR-2020 10:35:43

Comment           = Bs-HITAB
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 6[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.74587904[s]
Temp_get          = 22.6[dC]
```

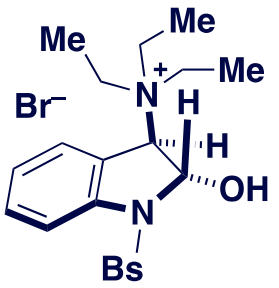


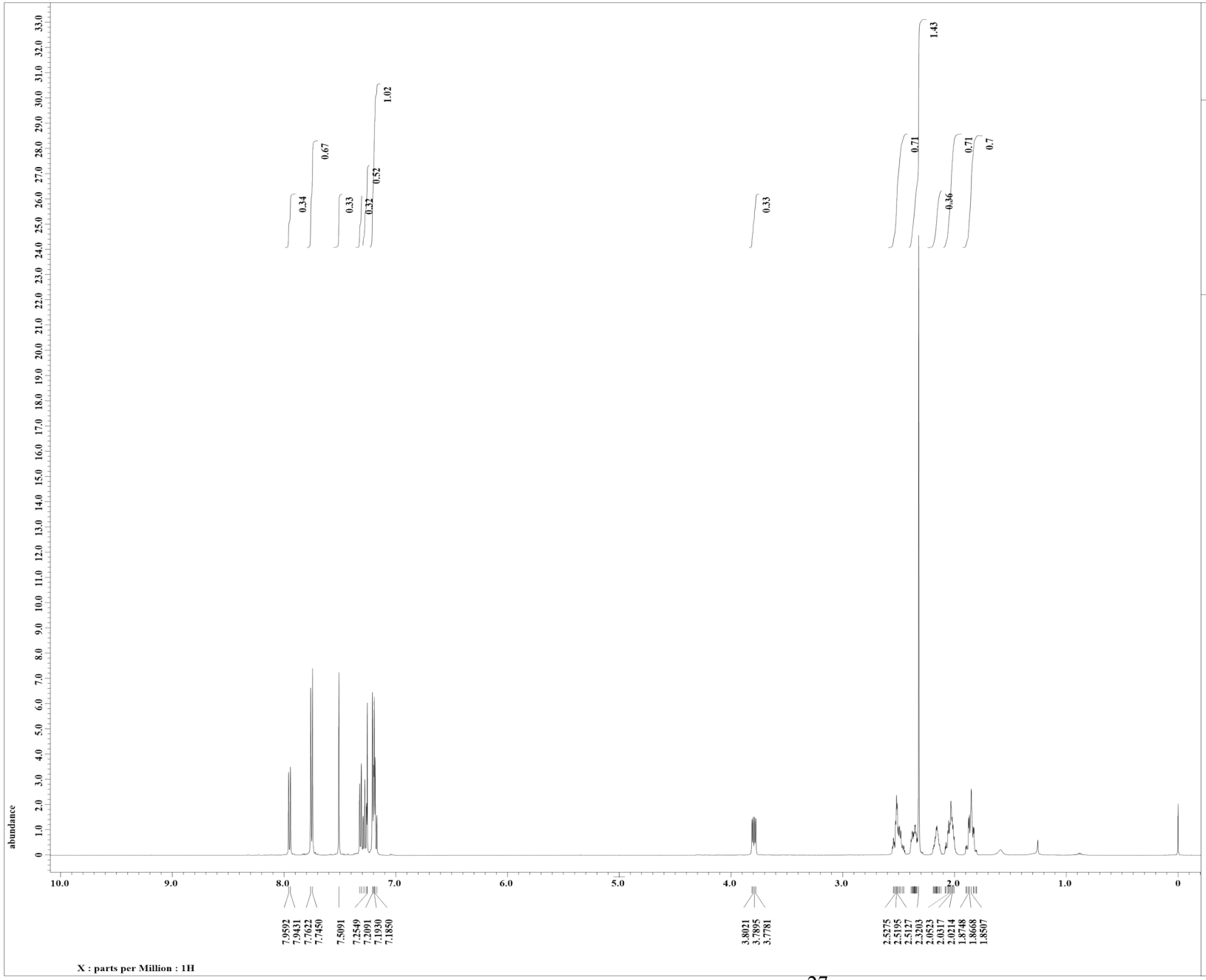



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA200414-1.jdf
```



```
Filename          = TA200414-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#567603
Solvent           = DMSO-D6
Creation_time     = 15-APR-2020 07:20:27
Revision_time     = 15-APR-2020 07:58:28
Current_time      = 15-APR-2020 07:59:51

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 20531
Total_scans       = 20531

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
RecVr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 24.1[dC]
```

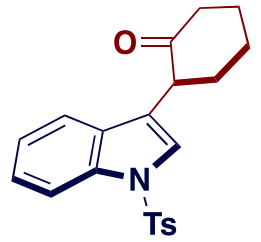



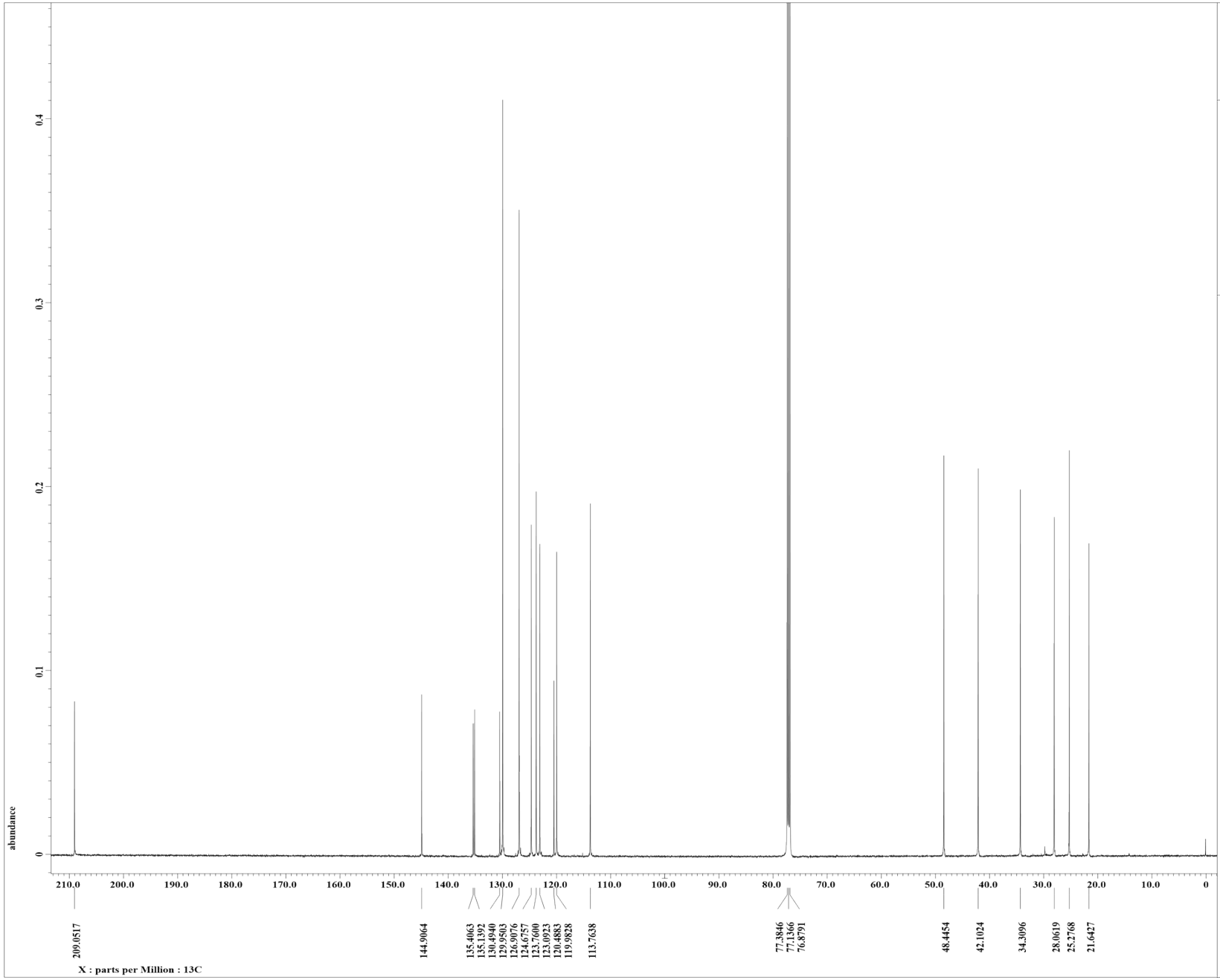


JEOL

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2019-0921-1.jdf
```

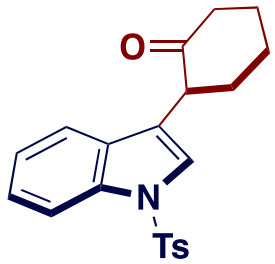
Filename	= TA2019-0921-7.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#626565
Solvent	= CHLOROFORM-D
Creation_time	= 21-SEP-2019 17:16:56
Revision_time	= 3-FEB-2020 18:51:21
Current_time	= 3-FEB-2020 18:52:40
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= TRUE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 12[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 5[s]
Repetition_time	= 6.74587904[s]
Temp_get	= 22.5[dC]

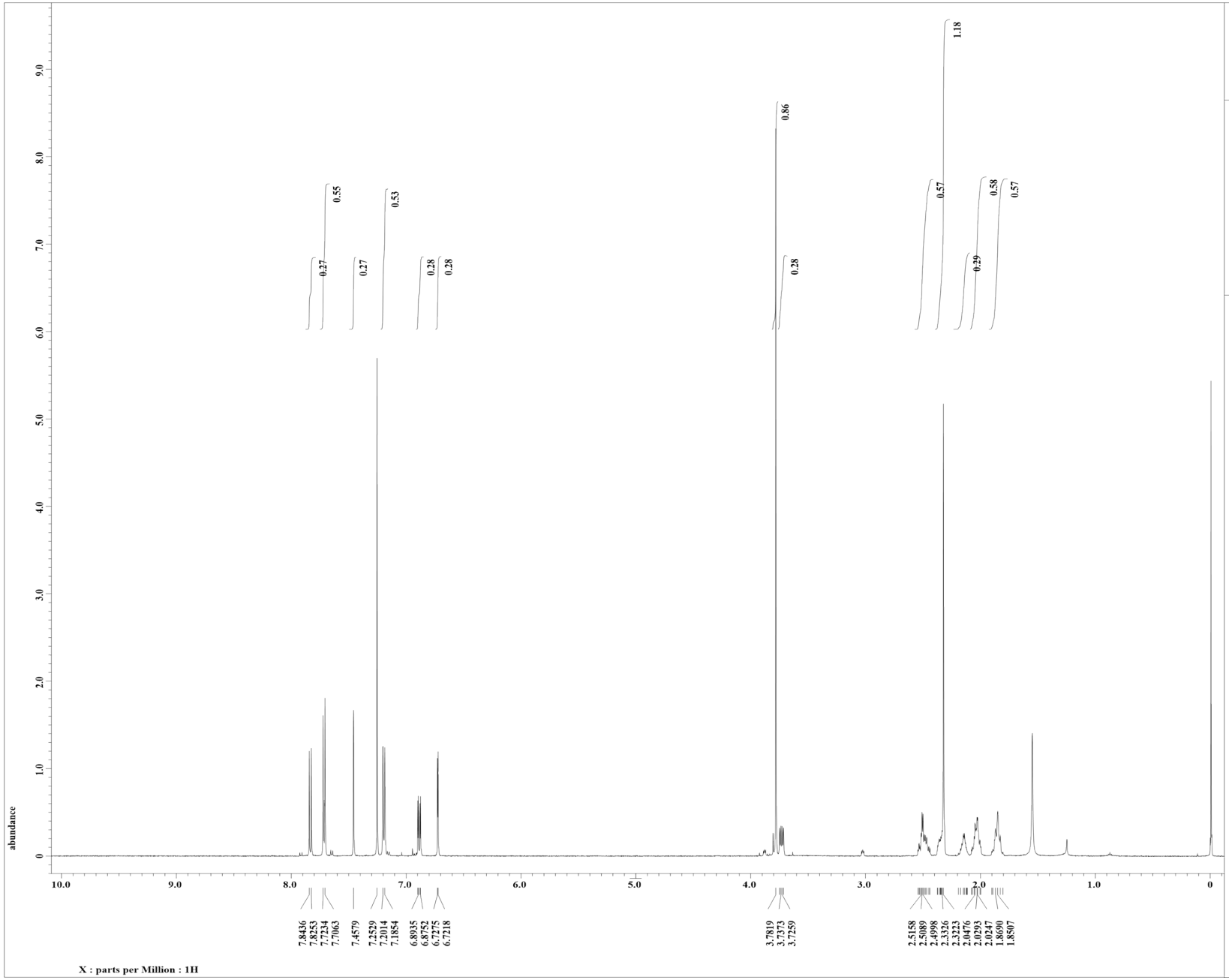




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2019-0921-2.jdf
```

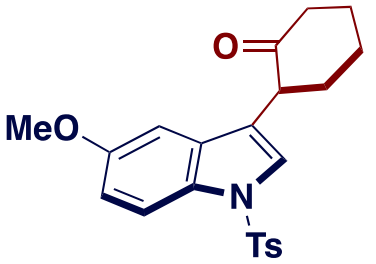
Filename	= TA2019-0921-6.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#627576
Solvent	= CHLOROFORM-D
Creation_time	= 24-SEP-2019 07:43:06
Revision_time	= 7-MAY-2020 15:26:58
Current_time	= 7-MAY-2020 15:27:46
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 79296
Total_scans	= 79296
X_90_width	= 12.8[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 5.3[dB]
X_pulse	= 4.26666667[us]
Irr_atn_dec	= 21.09[dB]
Irr_atn_noe	= 21.09[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 56
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 21.4[dC]

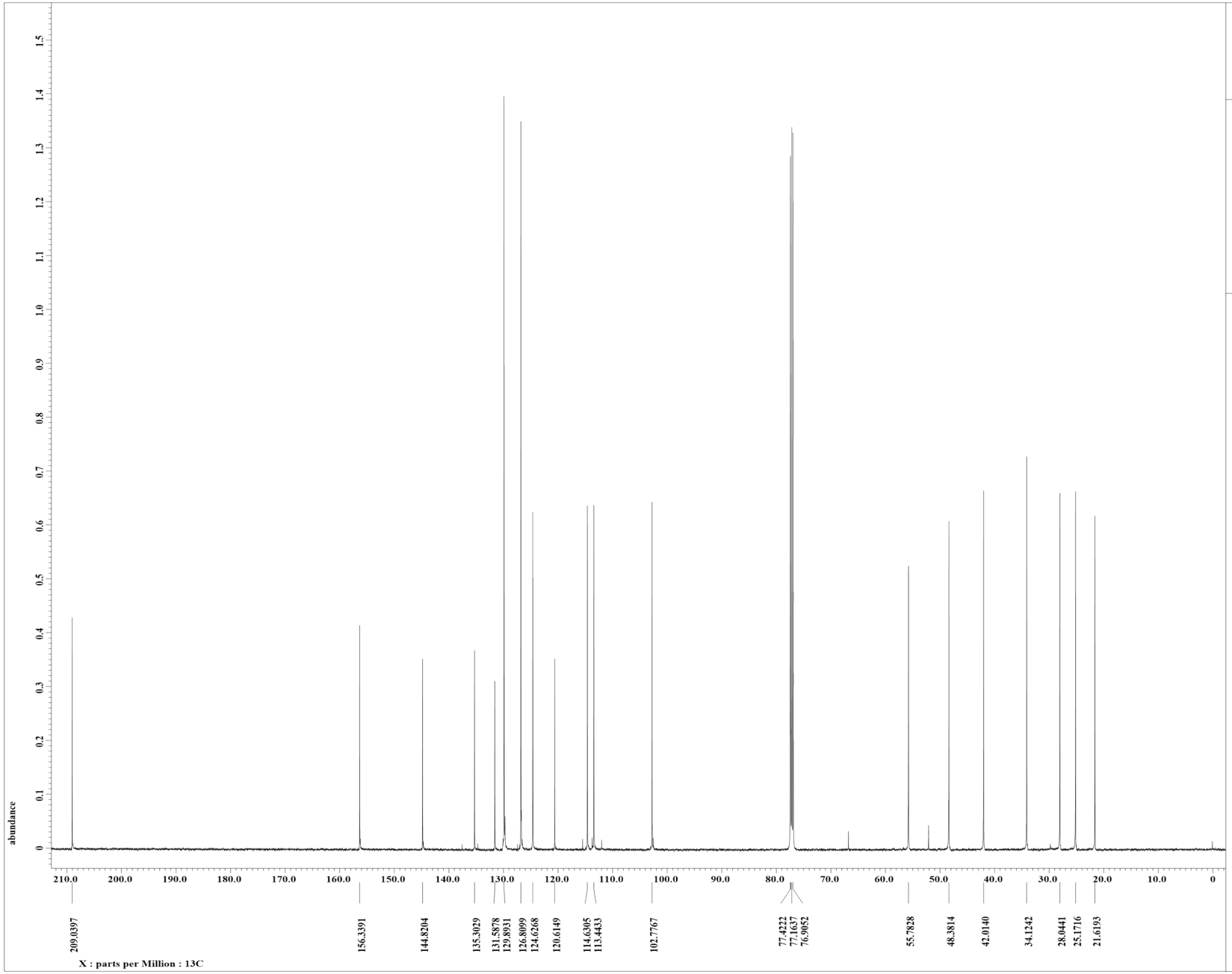




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA191016-1.jdf
```

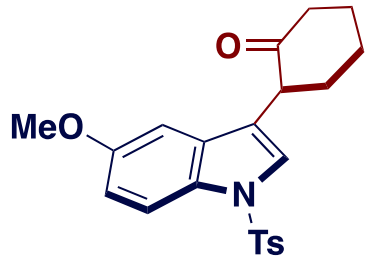
Filename	= TA191016-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#313594
Solvent	= CHLOROFORM-D
Creation_time	= 16-OCT-2019 08:05:07
Revision_time	= 8-MAY-2020 08:07:40
Current_time	= 8-MAY-2020 08:08:04
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 1.76422912[s]
X_domain	= 1H
X_freq	= 495.13191398[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.5668198[Hz]
X_sweep	= 9.28677563[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 495.13191398[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 11.3[us]
X_acq_time	= 1.76422912[s]
X_angle	= 45[deg]
X_atn	= 3.3[dB]
X_pulse	= 5.65[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 5[s]
Repetition_time	= 6.76422912[s]
Temp_get	= 23.8[dC]

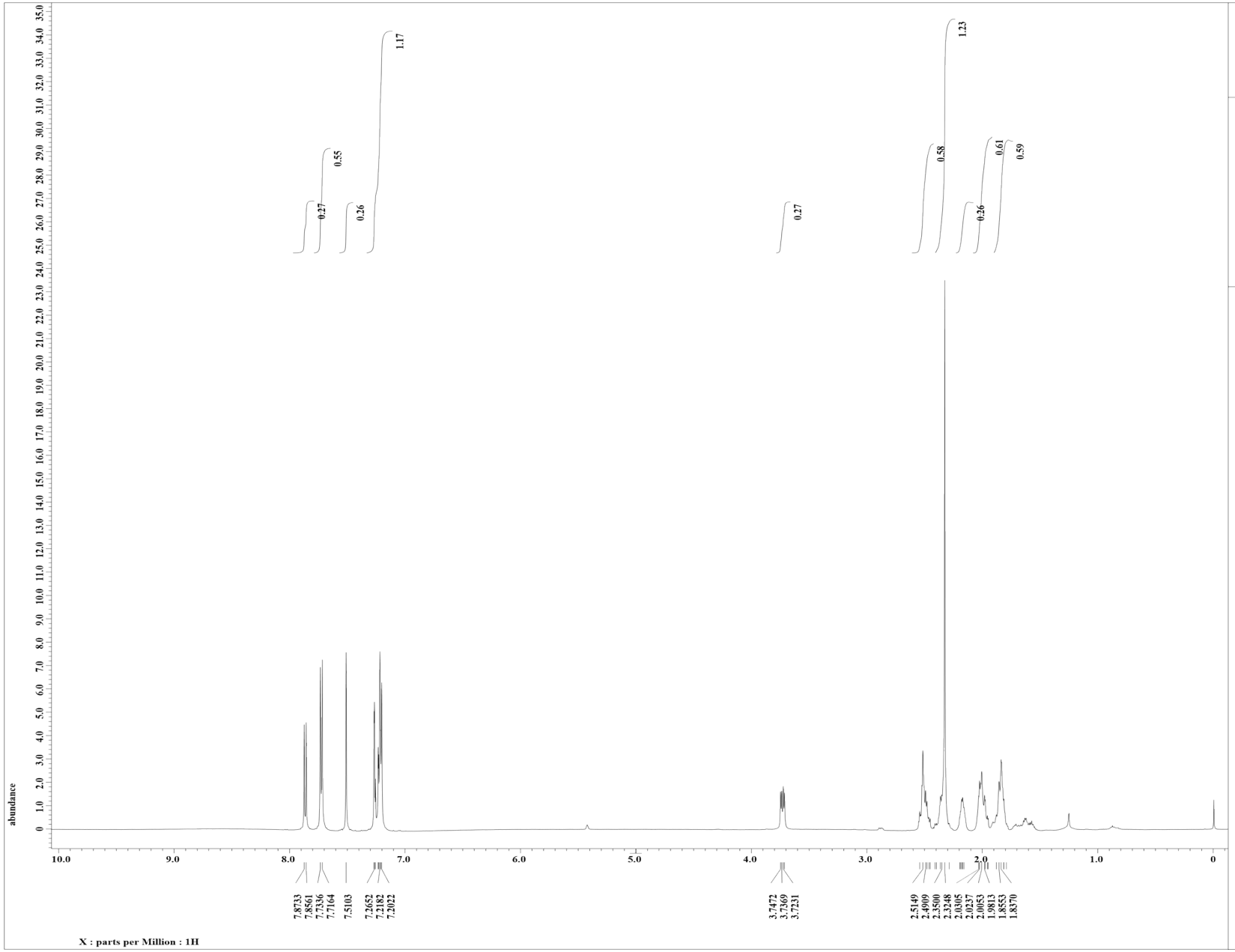


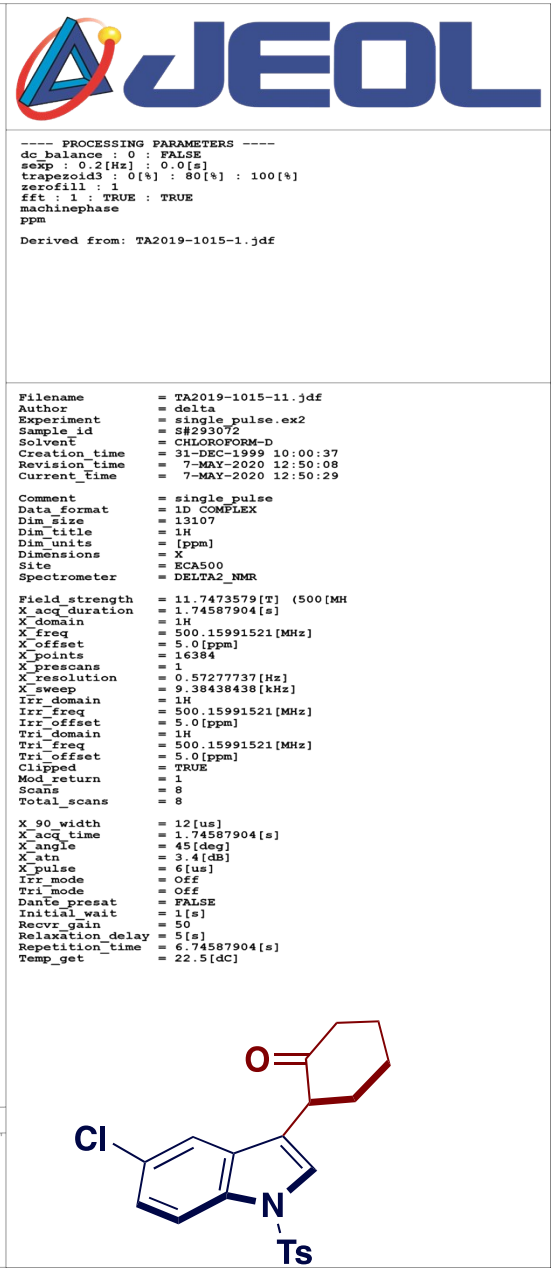


```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

Filename	= TA191015-12.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#684601
Solvent	= CHLOROFORM-D
Creation_time	= 16-OCT-2019 07:49:31
Revision_time	= 7-MAY-2020 15:53:18
Current_time	= 7-MAY-2020 15:53:59
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.5010059[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.1920929[Hz]
X_sweep	= 39.0625[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 17044
Total_scans	= 17044
X_90_width	= 10.1[us]
X_acq_time	= 0.8388608[s]
X_angle	= 30[deg]
X_atn	= 9.5[dB]
X_pulse	= 3.36666667[us]
Irr_atn_dec	= 21.51[dB]
Irr_atn_noe	= 21.51[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.8388608[s]
Temp_get	= 24.4[dC]

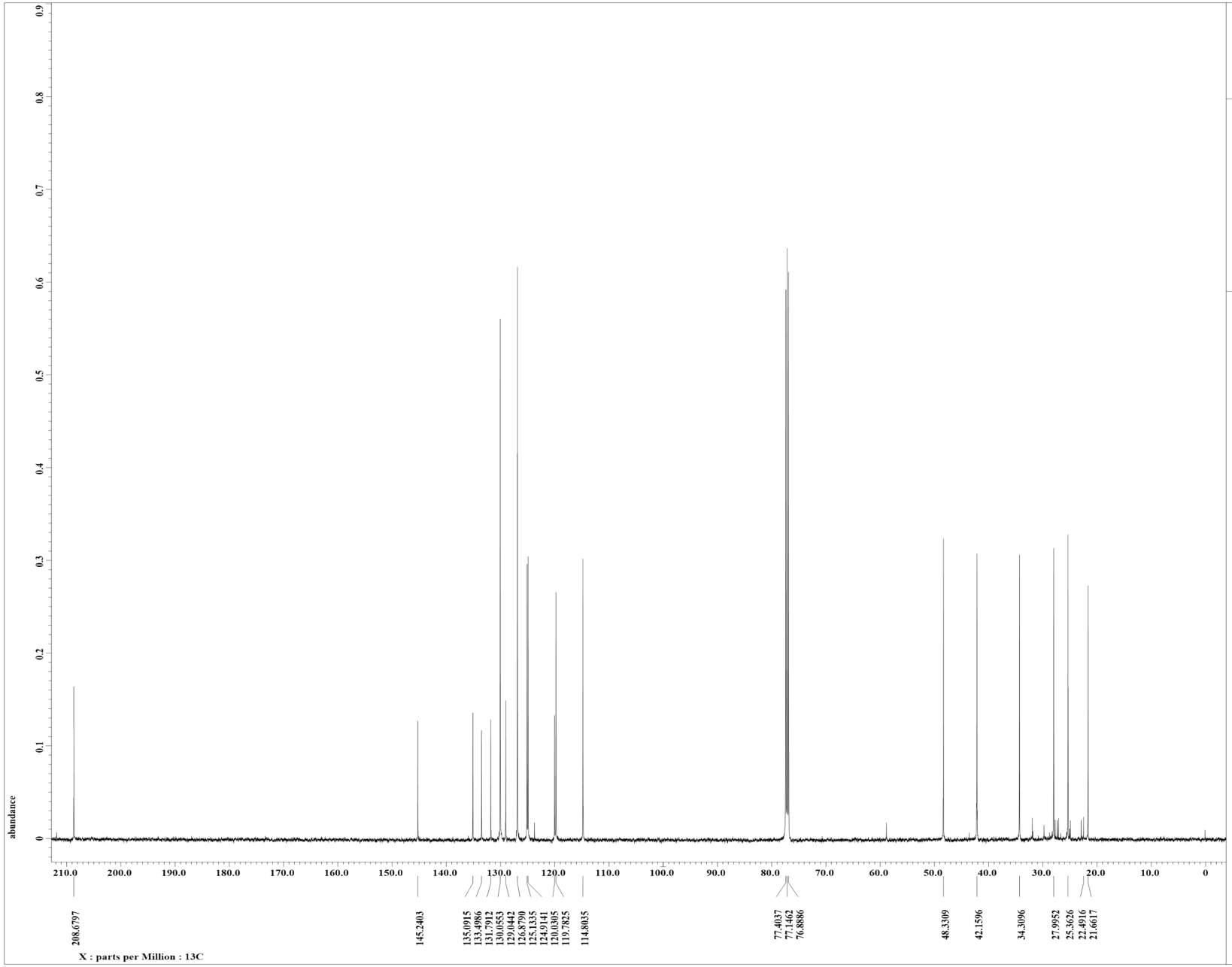






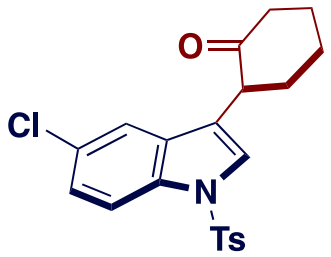

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2019-1015-1.jdf
```

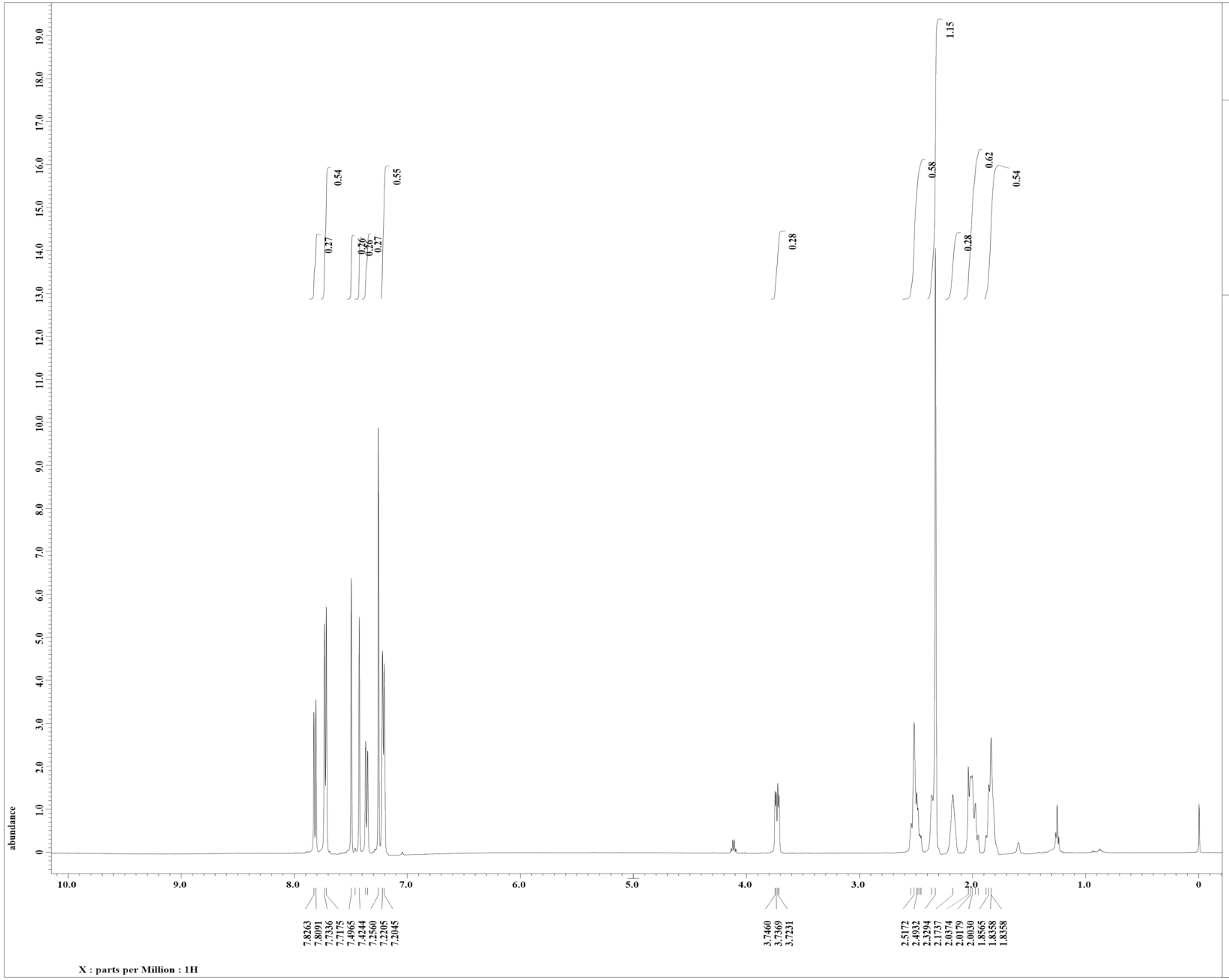
```
Filename          = TA2019-1015-11.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#293072
Solvent           = CHLOROFORM-D
Creation_time     = 31-DEC-1999 10:00:37
Revision_time     =  7-MAY-2020 12:50:08
Current_time      =  7-MAY-2020 12:50:29

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T]  (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 6[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.74587904[s]
Temp_get          = 22.5[dC]
```




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2019-1015-5.jdf
```

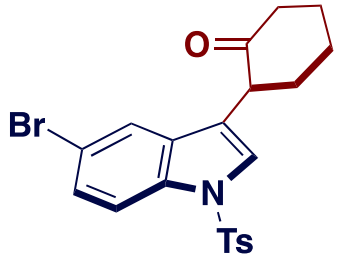
```
Filename            = TA2019-1015-11.jdf
Author              = delta
Experiment          = single_pulse_dec
Sample_id           = S#294065
Solvent             = CHLOROFORM-D
Creation_time       = 31-DEC-1999 12:38:32
Revision_time       =  7-MAY-2020 12:46:17
Current_time        =  7-MAY-2020 12:46:57

Comment             = single pulse decouple
Data_format         = 1D COMPLEX
Dim_size            = 26214
Dim_title           = 13C
Dim_units           = [ppm]
Dimensions          = X
Site                = ECA500
Spectrometer        = DELTA2_NMR

Field_strength      = 11.7473579[T] (500[MH
X_acq_duration      = 0.83361792[s]
X_domain            = 13C
X_freq              = 125.76529768[MHz]
X_offset            = 100[ppm]
X_points            = 32768
X_prescans          = 4
X_resolution        = 1.19959034[Hz]
X_sweep             = 39.3081761[kHz]
Irr_domain          = 1H
Irr_freq            = 500.15991521[MHz]
Irr_offset          = 5.0[ppm]
Clipped             = FALSE
Mod_return          = 1
Scans               = 3318
Total_scans         = 3318

X_90_width          = 12.8[us]
X_acq_time          = 0.83361792[s]
X_angle             = 30[deg]
X_atn               = 5.3[dB]
X_pulse             = 4.26666667[us]
Irr_atn_dec         = 21.09[dB]
Irr_atn_noe         = 21.09[dB]
Irr_noise           = WALTZ
Decoupling          = TRUE
Initial_wait        = 1[s]
Noe                 = TRUE
Noe_time            = 2[s]
Recvr_gain          = 58
Relaxation_delay    = 2[s]
Repetition_time     = 2.83361792[s]
Temp_get            = 23.4[dC]
```

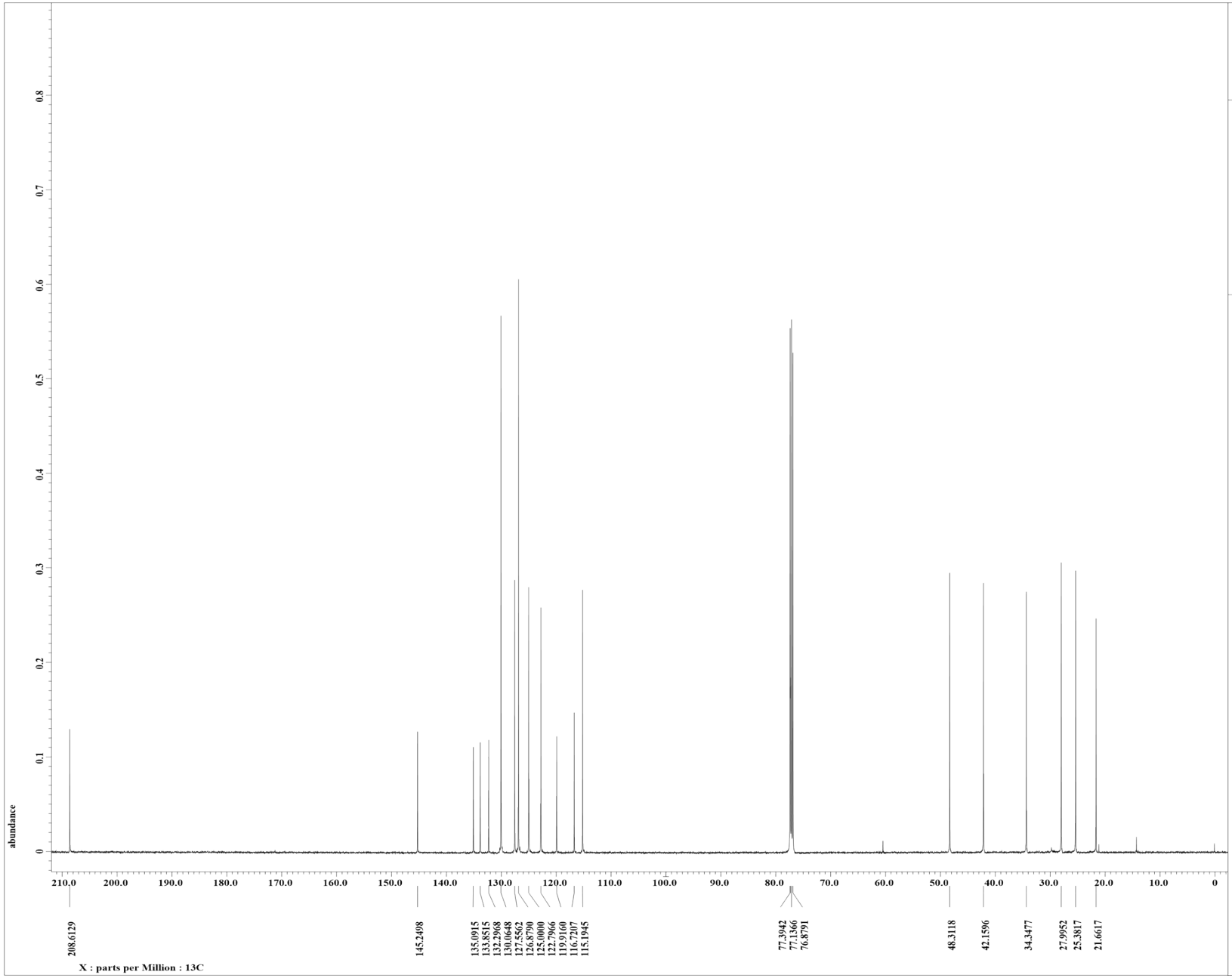


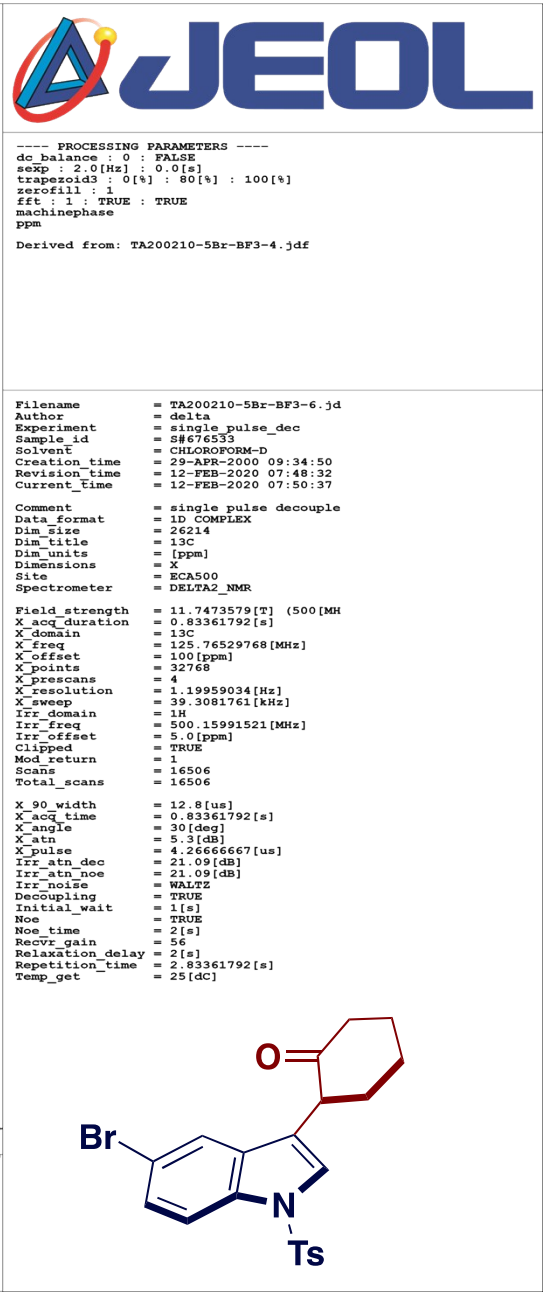


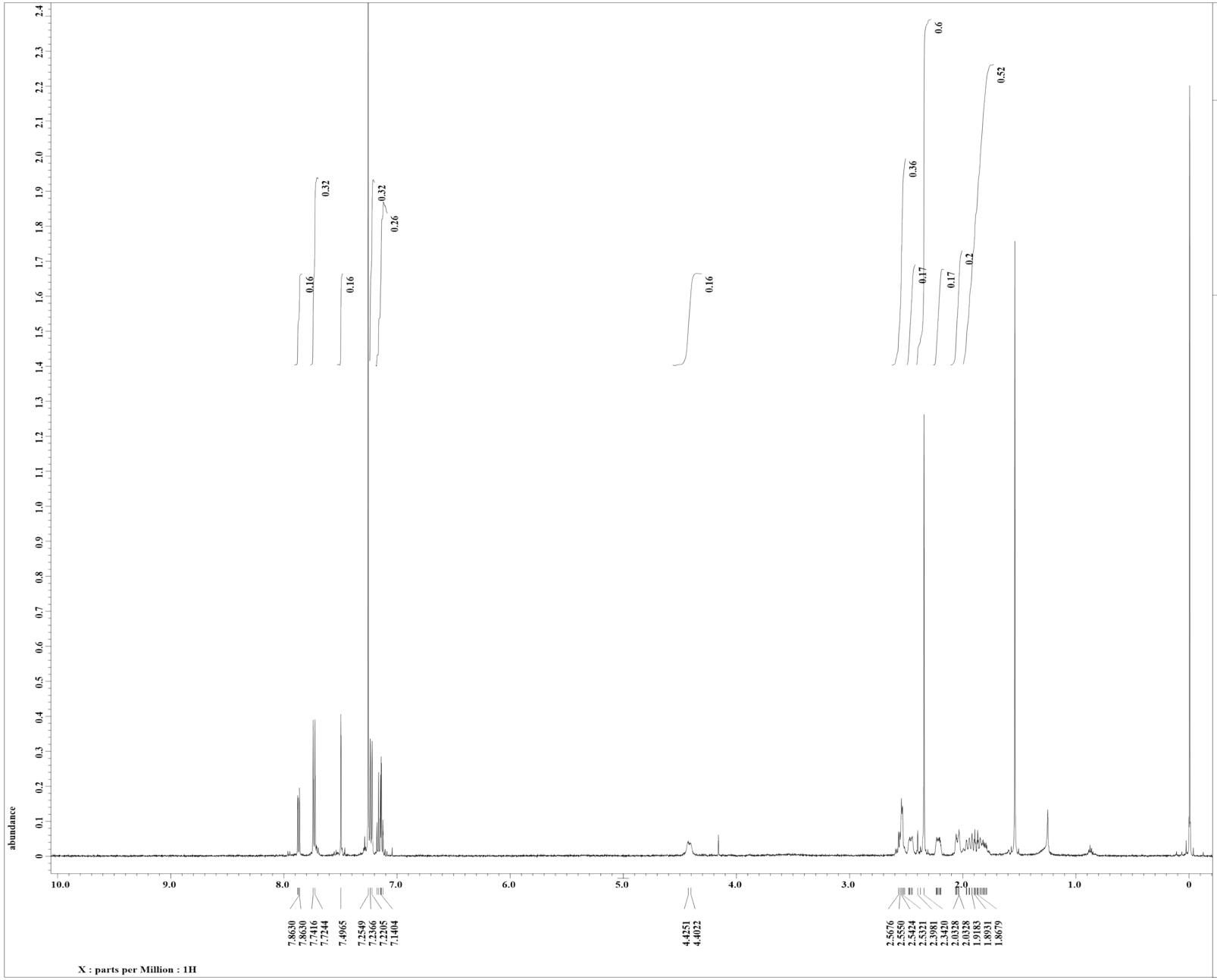

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA200210-5Br-BF3-2.jdf
```

Filename	= TA200210-5Br-BF3-5.jd
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#675746
Solvent	= CHLOROFORM-D
Creation_time	= 28-APR-2000 20:34:21
Revision_time	= 12-FEB-2020 07:56:58
Current_time	= 12-FEB-2020 07:57:46
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= TRUE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 12[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 5[s]
Repetition_time	= 6.74587904[s]
Temp_get	= 23[dC]



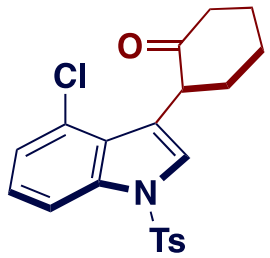

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
208.6129
145.2498
135.0915
133.8515
132.2968
130.0648
127.5562
126.8790
125.0000
122.7966
119.9160
116.7207
115.1945
77.3942
77.1366
76.8791
48.3118
42.1596
34.3477
27.9952
25.3817
21.6617
X : parts per Million : 13C

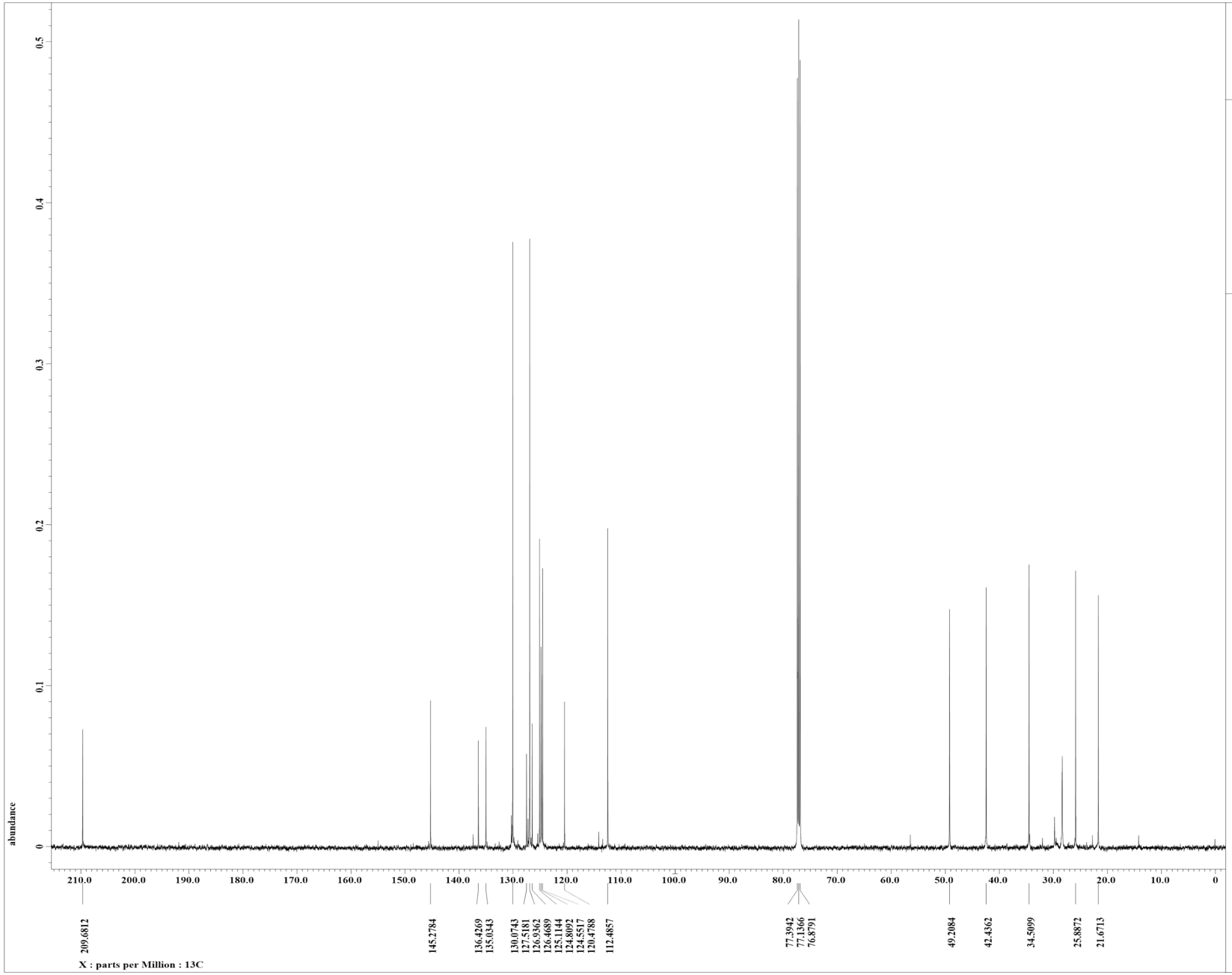

JEOL
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: TA200210-5Br-BF3-4.jdf
Filename = TA200210-5Br-BF3-6.jd
Author = delta
Experiment = single_pulse_dec
Sample_id = S#676533
Solvent = CHLOROFORM-D
Creation_time = 29-APR-2000 09:34:50
Revision_time = 12-FEB-2020 07:48:32
Current_time = 12-FEB-2020 07:50:37
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034[Hz]
X_sweep = 39.3081761[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 16506
Total_scans = 16506
X_90_width = 12.8[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 5.3[dB]
X_pulse = 4.26666667[us]
Irr_atn_dec = 21.09[dB]
Irr_atn_noe = 21.09[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 56
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 25[dC]
O
Br
N
Ts



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA200306-4Cl-1.jdf
```

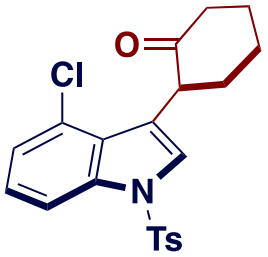
Filename	= TA200306-4Cl-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#387368
Solvent	= CHLOROFORM-D
Creation_time	= 22-MAY-2000 12:32:57
Revision_time	= 6-MAR-2020 10:55:26
Current_time	= 6-MAR-2020 10:55:44
Comment	= 4Cl-cyclohexanone
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 12[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 5[s]
Repetition_time	= 6.74587904[s]
Temp_get	= 22.2[dC]

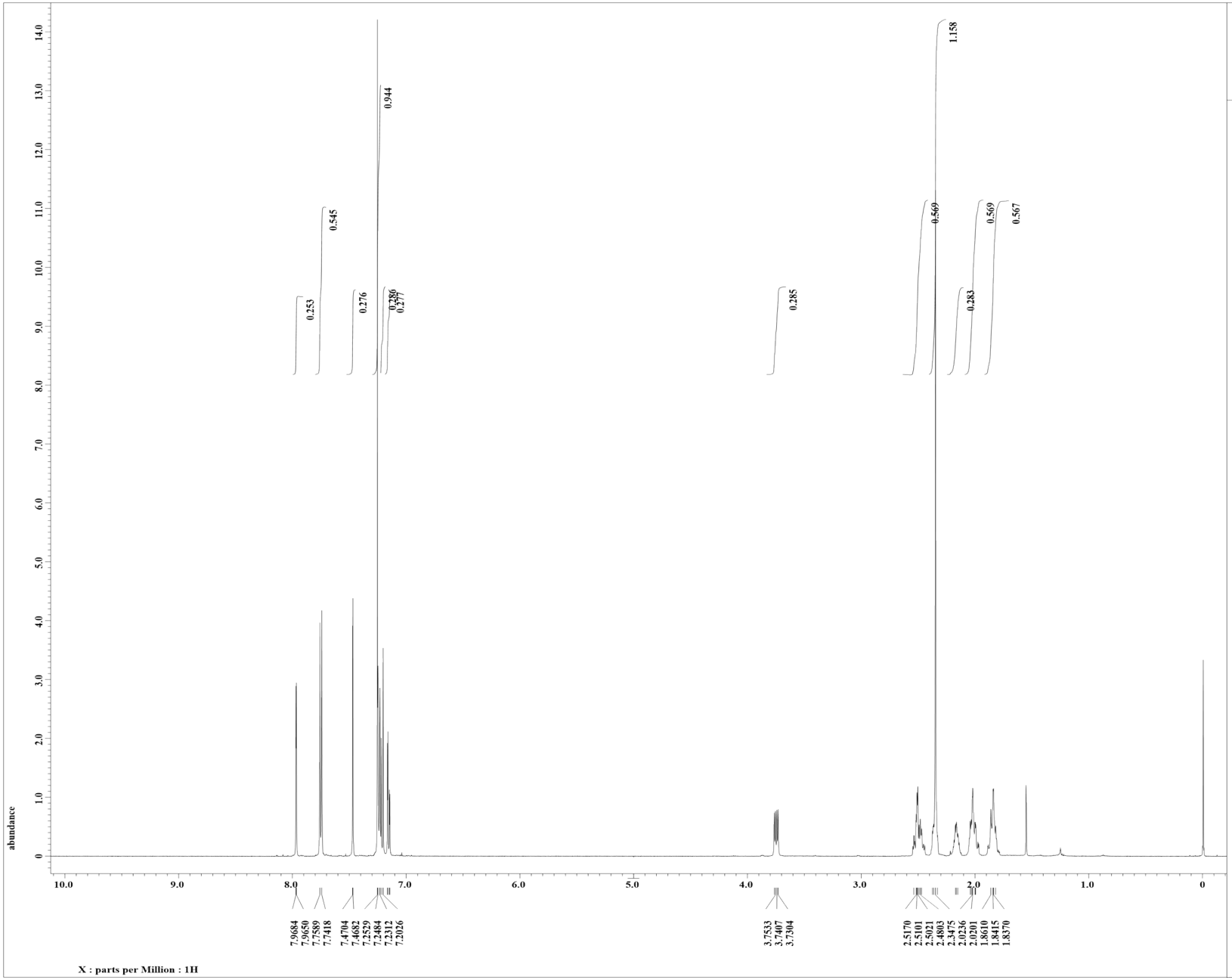





```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA200306-4Cl-2.jdf
```

```
Filename          = TA200306-4Cl-5.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#390459
Solvent           = CHLOROFORM-D
Creation_time     = 22-MAY-2000 14:47:07
Revision_time     =  6-MAR-2020 13:01:22
Current_time      =  6-MAR-2020 13:02:10

Comment           = 4Cl-cyclohexanone
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 2738
Total_scans       = 2738

X_90_width        = 12.8[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 5.3[dB]
X_pulse           = 4.26666667[us]
Irr_atn_dec       = 21.09[dB]
Irr_atn_noe       = 21.09[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 54
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 22.8[dC]
```



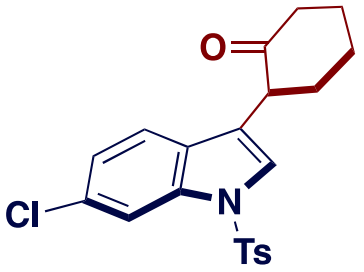


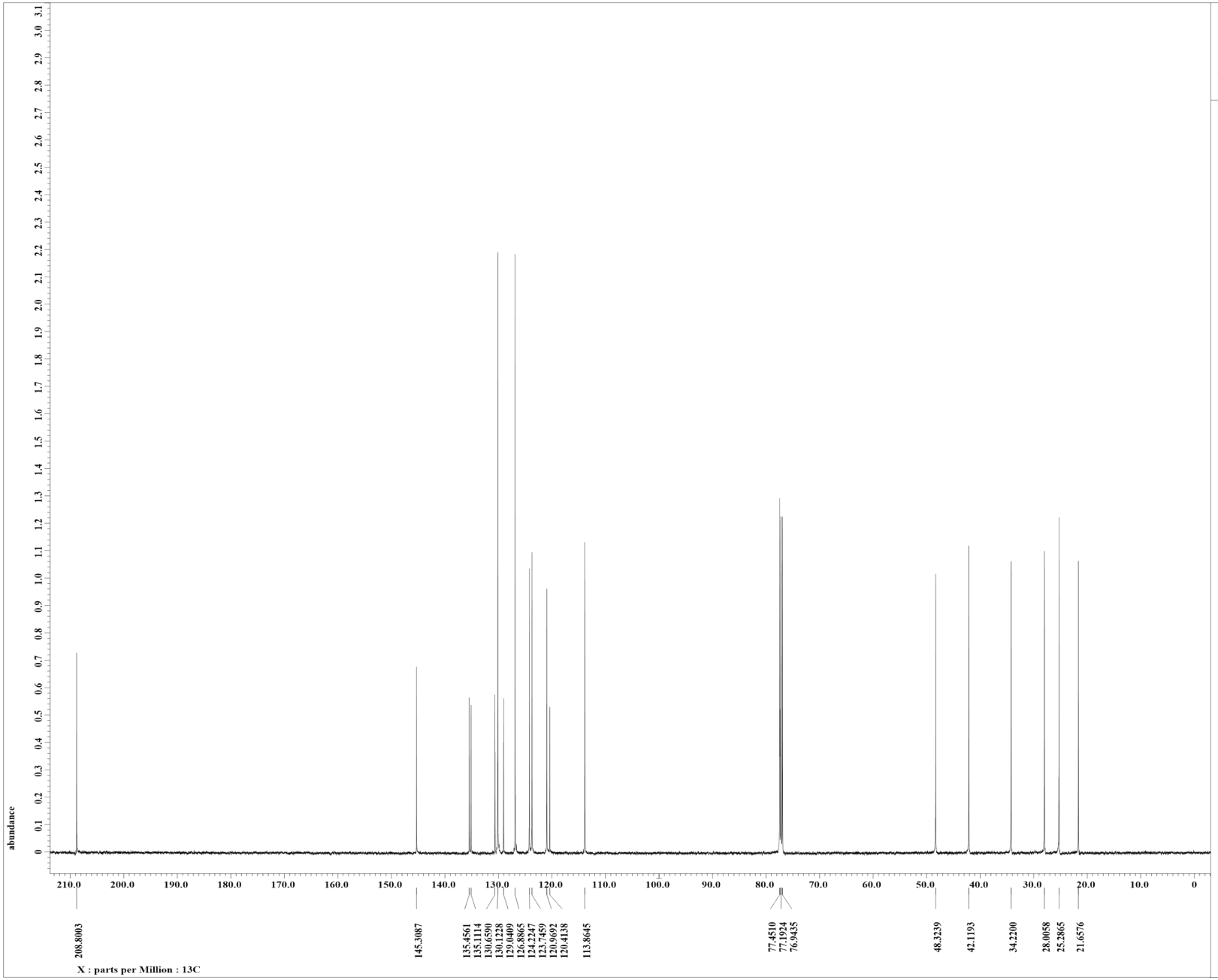
Filename = 6-Cl-Cyclohexanone-1H
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#597163
Solvent = CHLOROFORM-D
Creation_time = 27-FEB-2020 15:37:29
Revision_time = 27-FEB-2020 16:40:17
Current_time = 27-FEB-2020 16:41:01

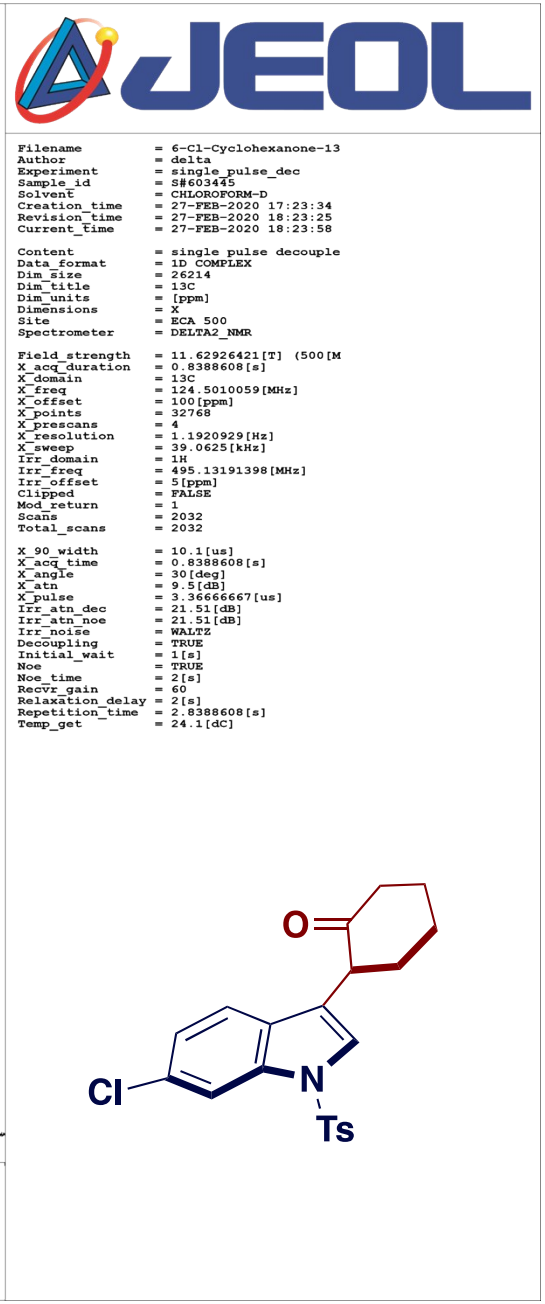
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.3[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_pulse = 5.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 48
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 23.4[dC]





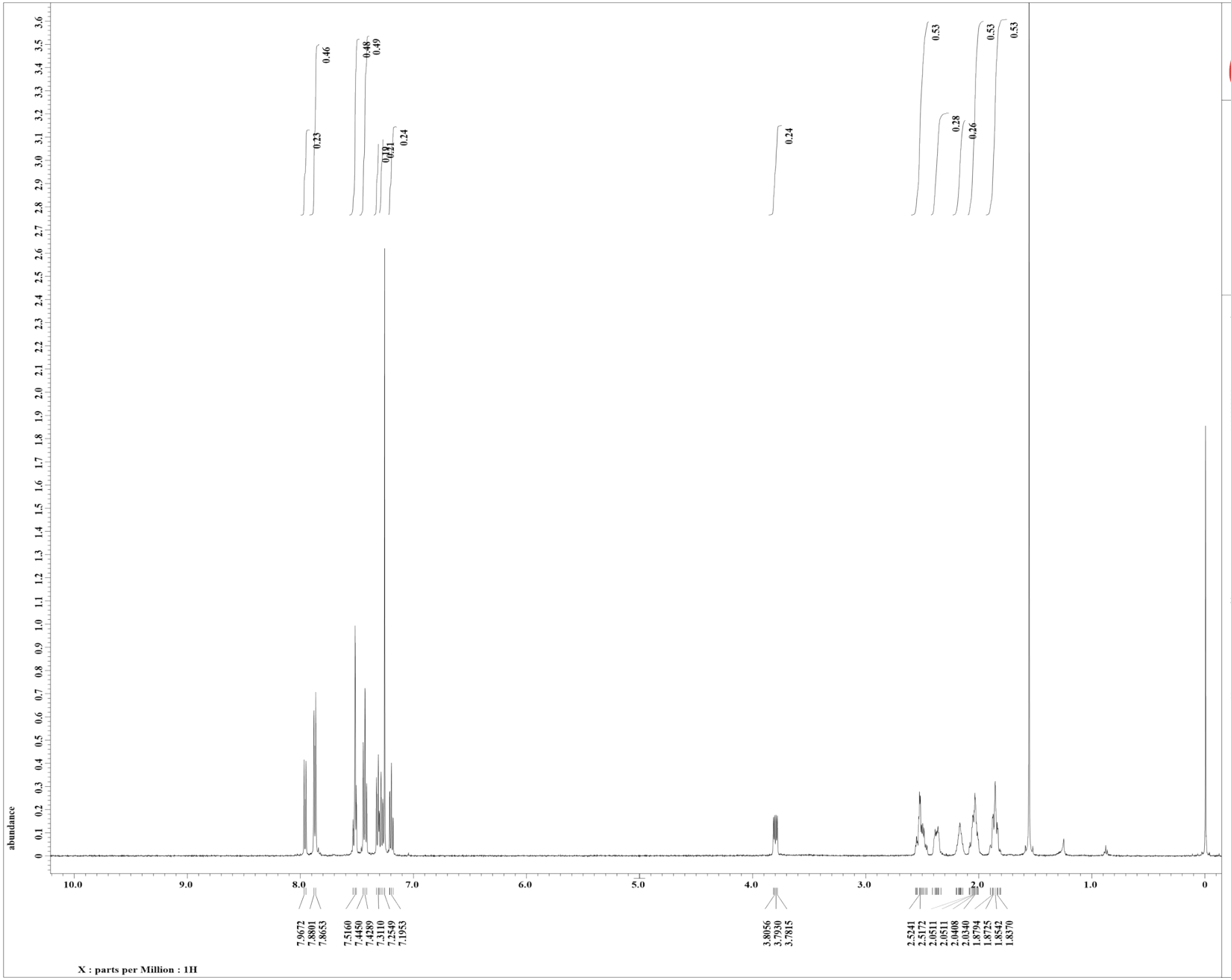


Filename = 6-Cl-Cyclohexanone-13
Author = delta
Experiment = single_pulse_dec
Sample_id = S#603445
Solvent = CHLOROFORM-D
Creation_time = 27-FEB-2020 17:23:34
Revision_time = 27-FEB-2020 18:23:25
Current_time = 27-FEB-2020 18:23:58

Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

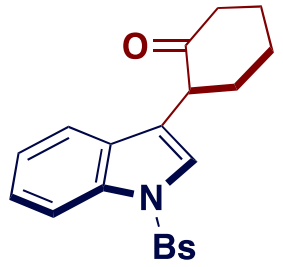
Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 2032
Total_scans = 2032

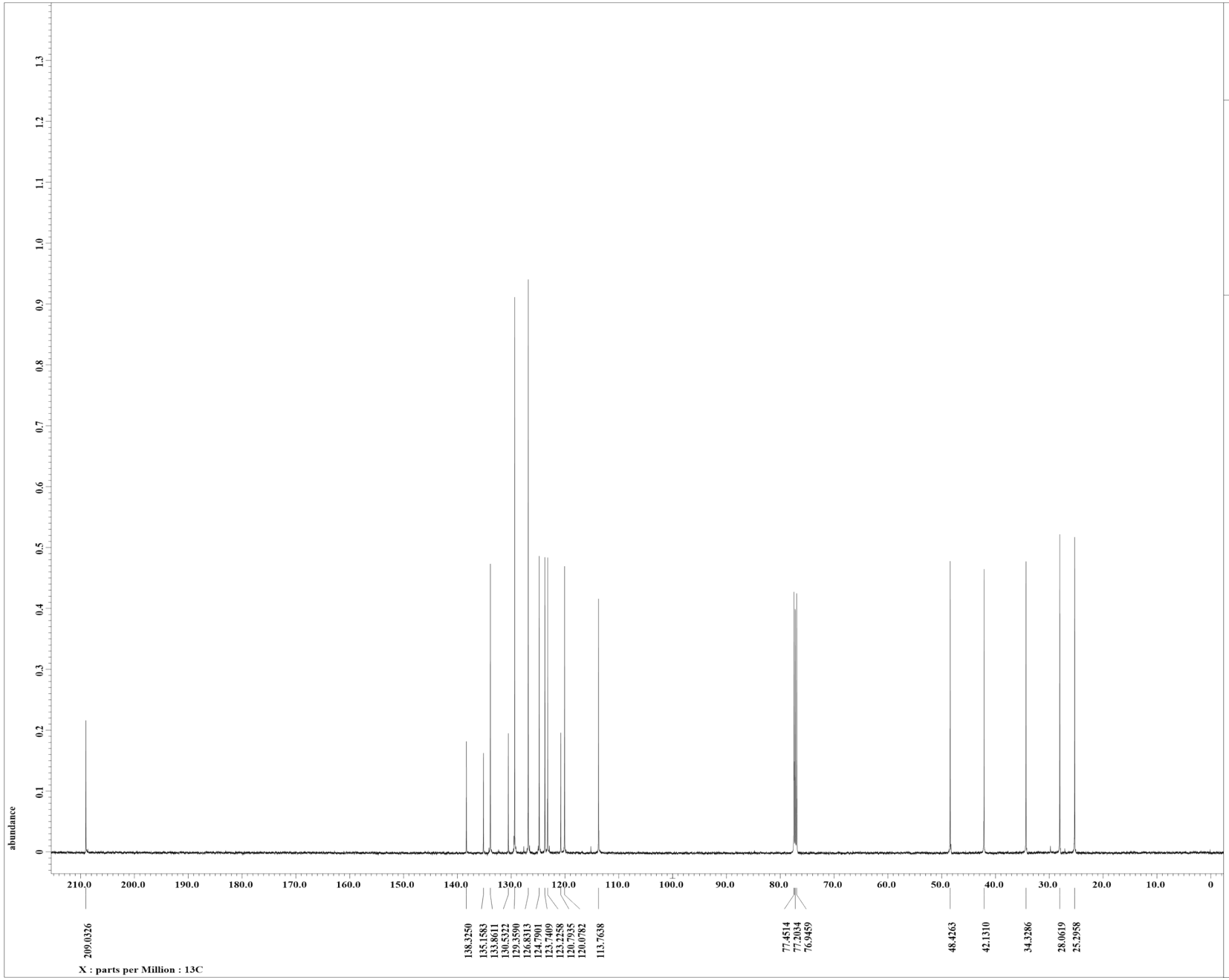
X_90_width = 10.1[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.36666667[us]
Irr_atn_dec = 21.51[dB]
Irr_atn_noe = 21.51[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get = 24.1[dC]




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA200515-2-1.jdf
```

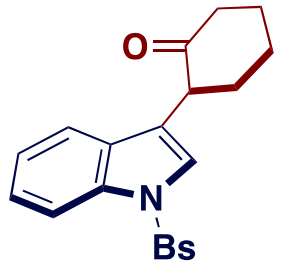
Filename	= TA200515-2-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#612538
Solvent	= CHLOROFORM-D
Creation_time	= 31-JUL-2000 18:45:50
Revision_time	= 15-MAY-2020 17:07:30
Current_time	= 15-MAY-2020 17:07:51
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 12[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 5[s]
Repetition_time	= 6.74587904[s]
Temp_get	= 21.8[dC]

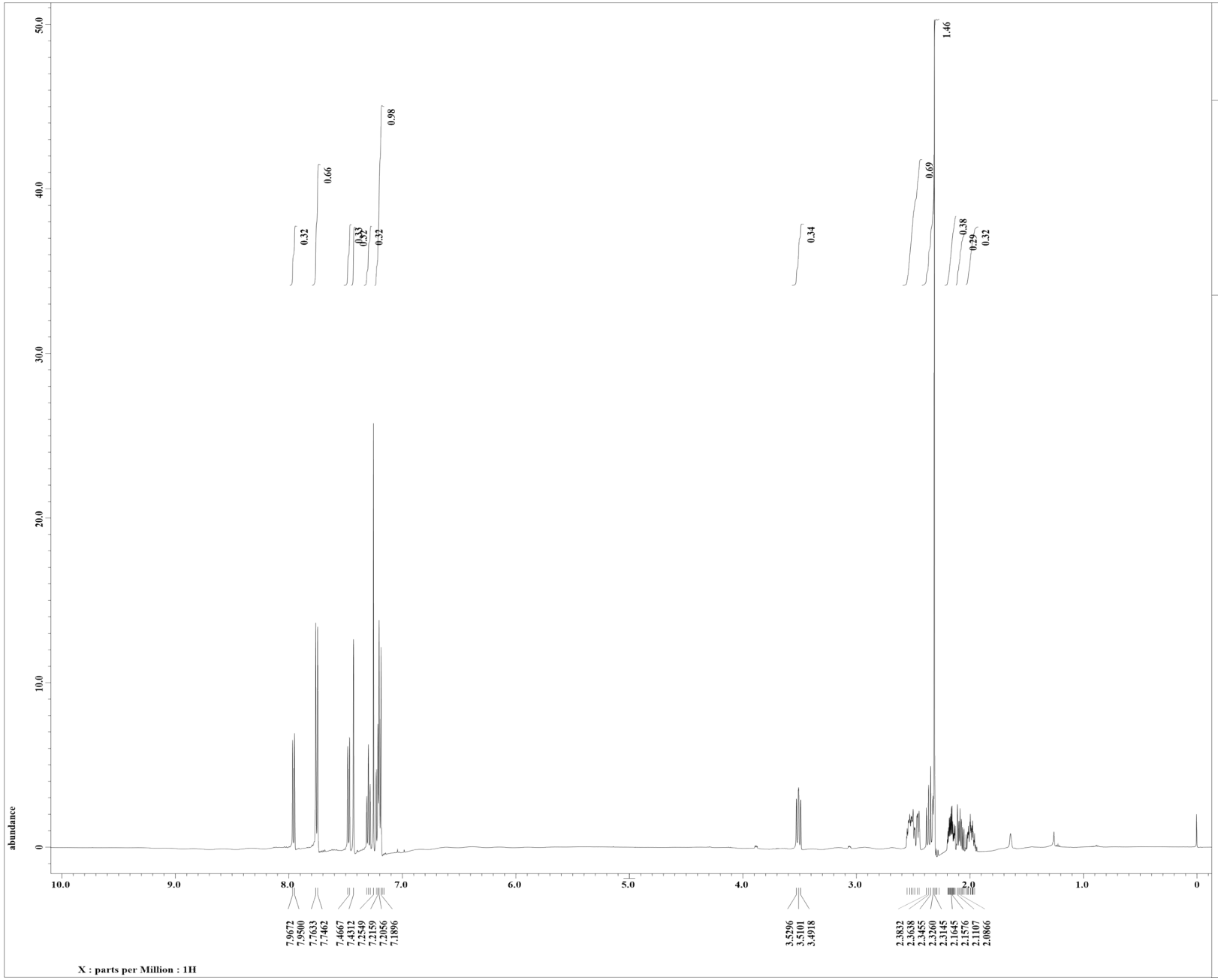





```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA200515-2-2.jdf
```

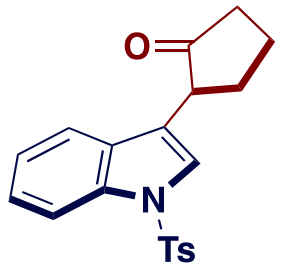
```
Filename          = TA200515-2-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#615617
Solvent           = CHLOROFORM-D
Creation_time     = 31-JUL-2000 20:21:58
Revision_time     = 15-MAY-2020 18:39:08
Current_time      = 15-MAY-2020 18:39:29

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1936
Total_scans       = 1936

X_90_width        = 12.8[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 5.3[dB]
X_pulse           = 4.26666667[us]
Irr_atn_dec       = 21.09[dB]
Irr_atn_noe       = 21.09[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 54
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 23.2[dC]
```

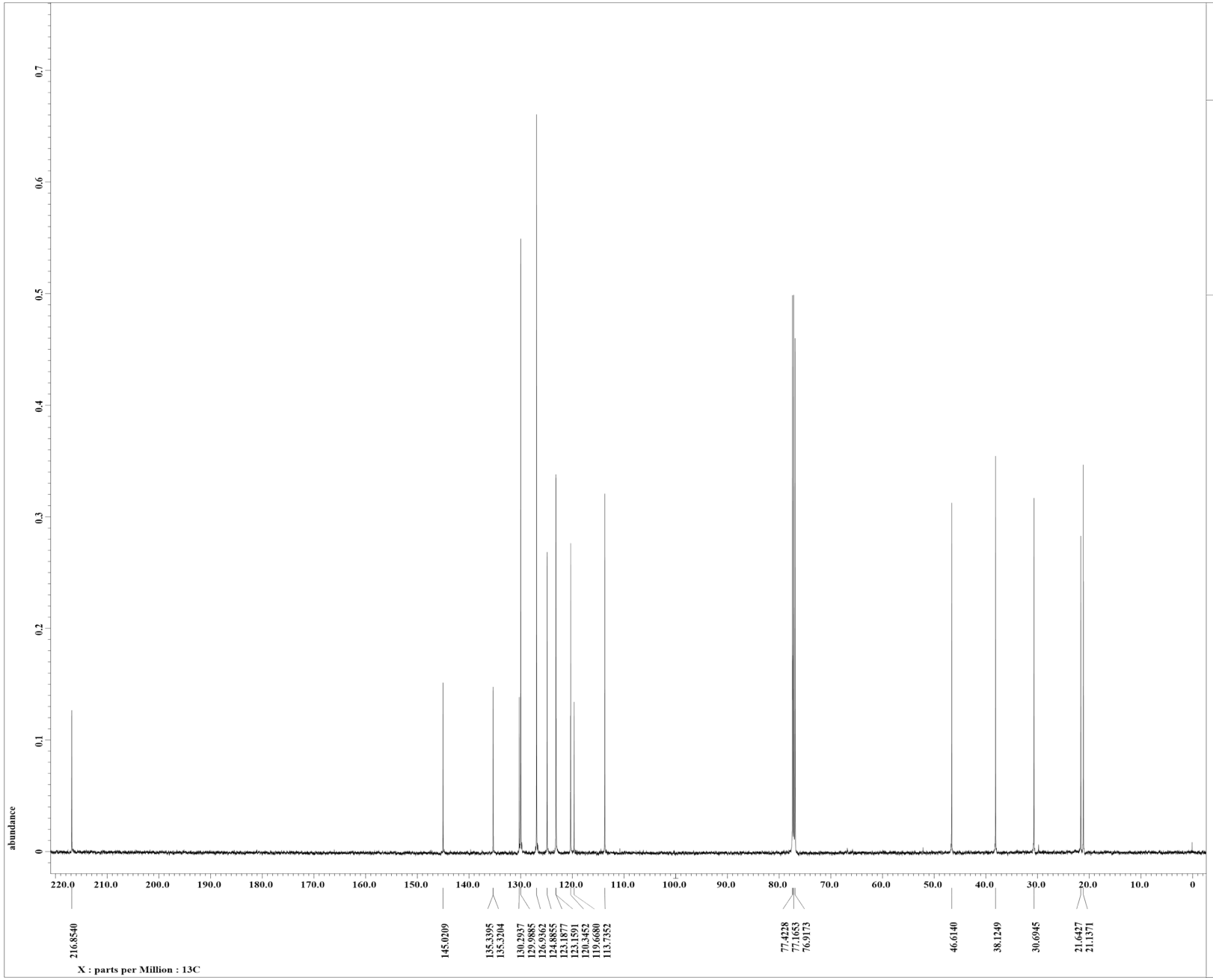






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2019-1007-7.jdf
```

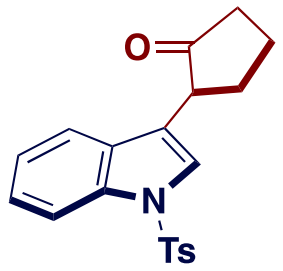
```
Filename          = TA2019-1007-17.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#472209
Solvent           = CHLOROFORM-D
Creation_time     =  7-OCT-2019 12:59:10
Revision_time     =  7-MAY-2020 13:03:36
Current_time      =  7-MAY-2020 13:04:02

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 6[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.74587904[s]
Temp_get          = 22.7[dC]
```

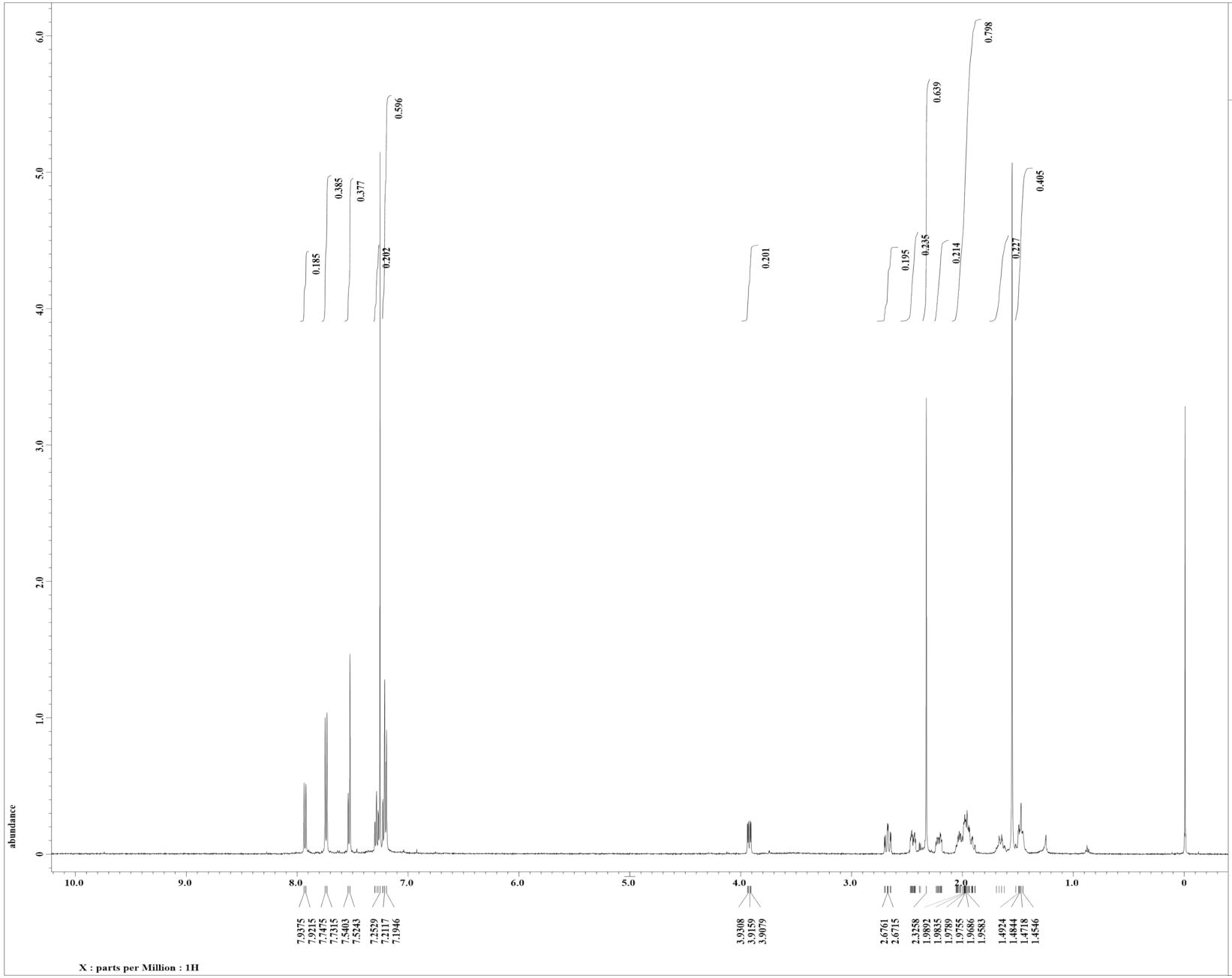




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2019-1007-15.jdf
```

```
Filename          = TA2019-1007-17.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#544196
Solvent           = CHLOROFORM-D
Creation_time     =  7-OCT-2019 16:53:46
Revision_time     =  7-MAY-2020 12:59:44
Current_time      =  7-MAY-2020 13:00:54

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 2437
Total_scans       = 2437

X_90_width        = 12.8[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 5.3[dB]
X_pulse           = 4.26666667[us]
Irr_atn_dec       = 21.09[dB]
Irr_atn_noe       = 21.09[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 54
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 22.3[dC]
```



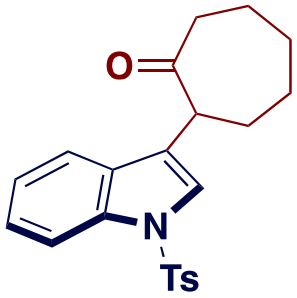


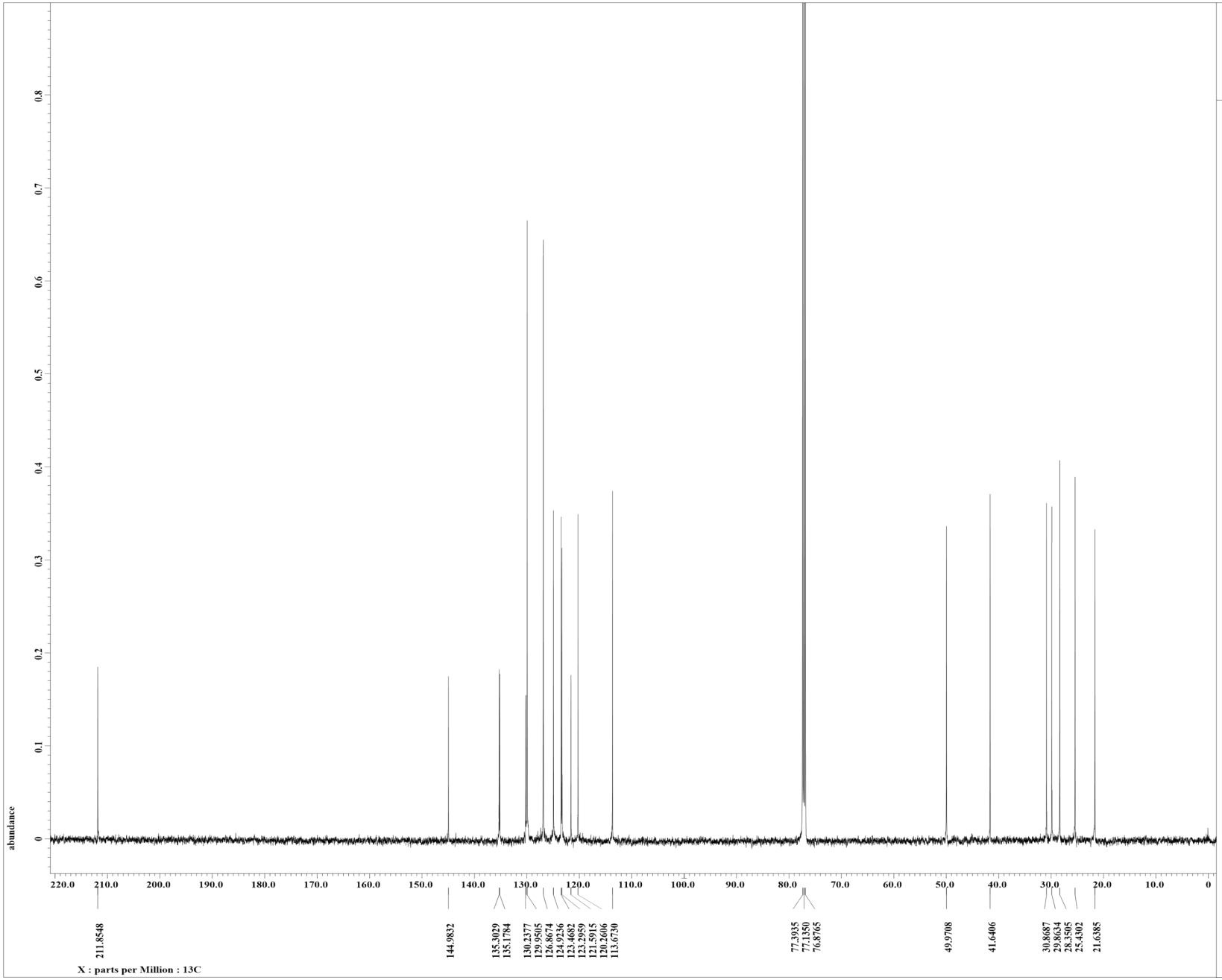
Filename = TA200529-cycloheptano
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#309246
Solvent = CHLOROFORM-D
Creation_time = 29-MAY-2020 07:56:51
Revision_time = 29-MAY-2020 08:43:07
Current_time = 29-MAY-2020 08:43:50

Content = cycloheptanone
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

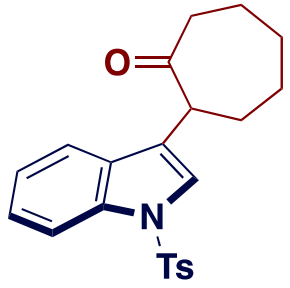
Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

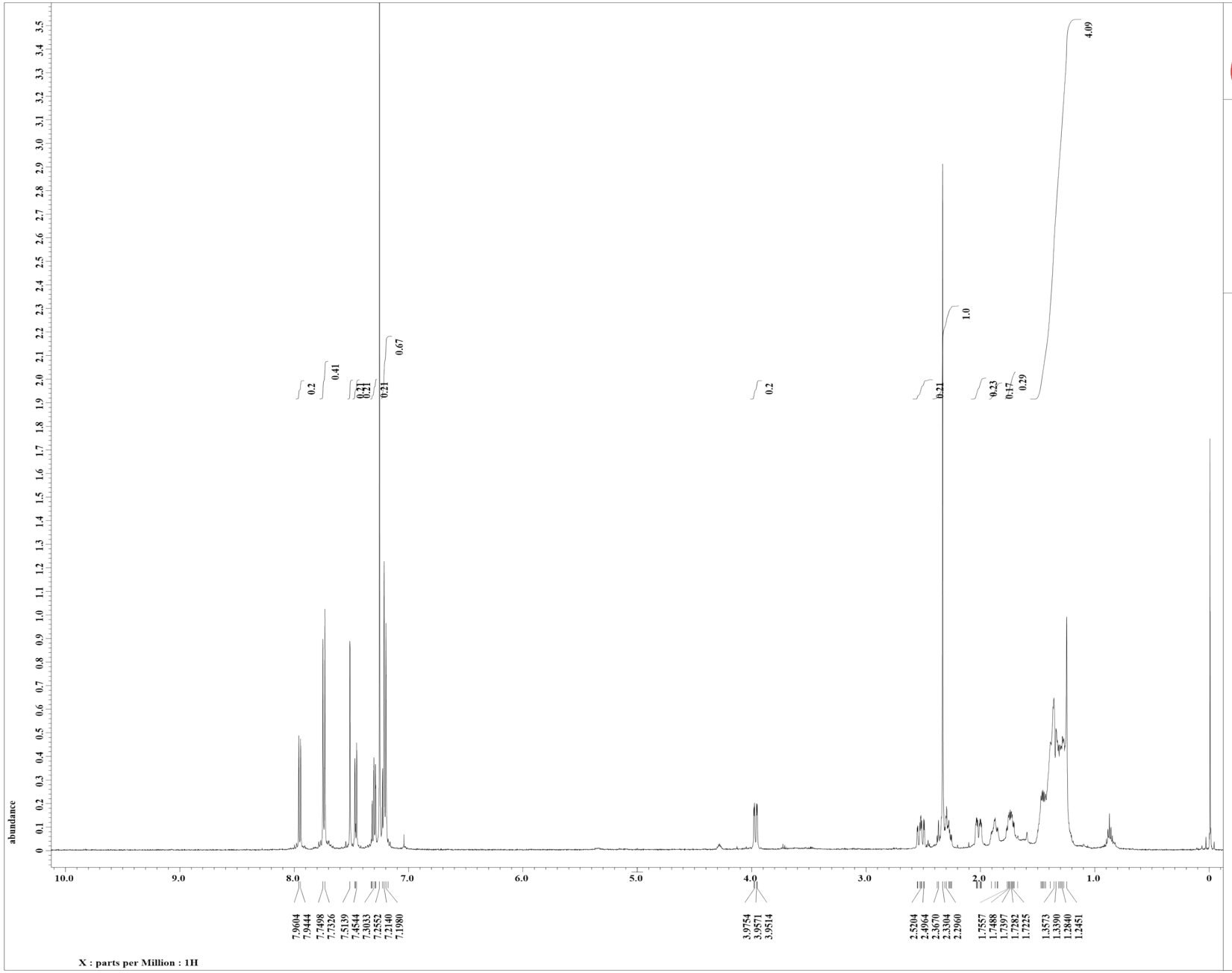
X_90_width = 11.3[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_pulse = 5.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 23.7[dC]

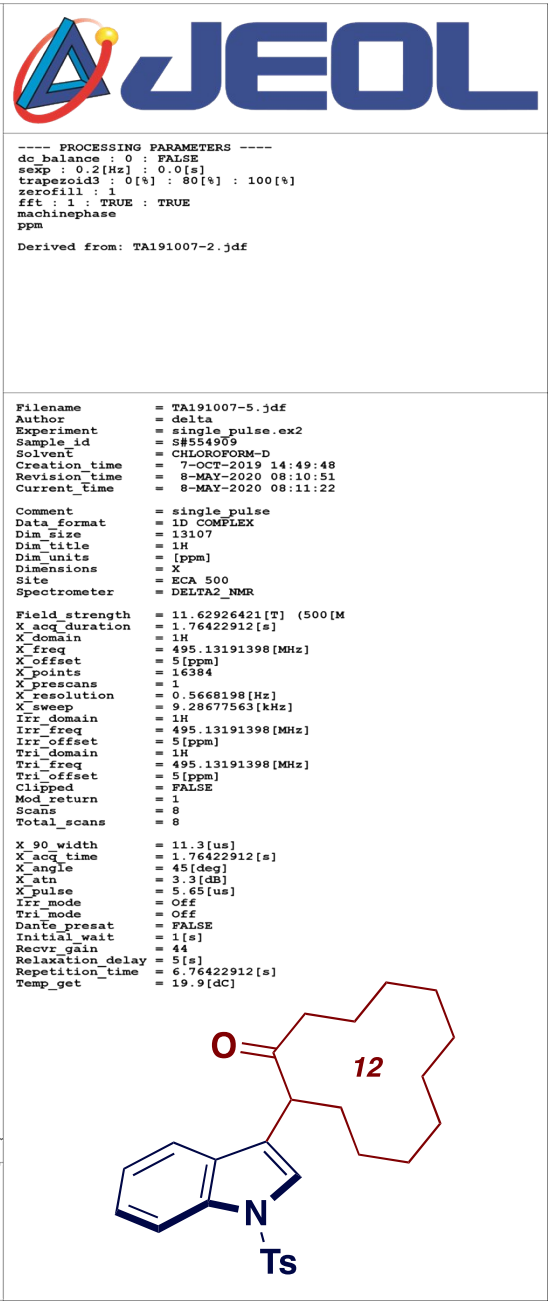




```
Filename          = TA200529-cycloheptano
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#312929
Solvent           = CHLOROFORM-D
Creation_time     = 29-MAY-2020 10:04:13
Revision_time     = 29-MAY-2020 10:44:32
Current_time      = 29-MAY-2020 10:45:14

Content           = cycloheptanone-13C
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 2568
Total_scans       = 2568

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 24.7[dC]
```

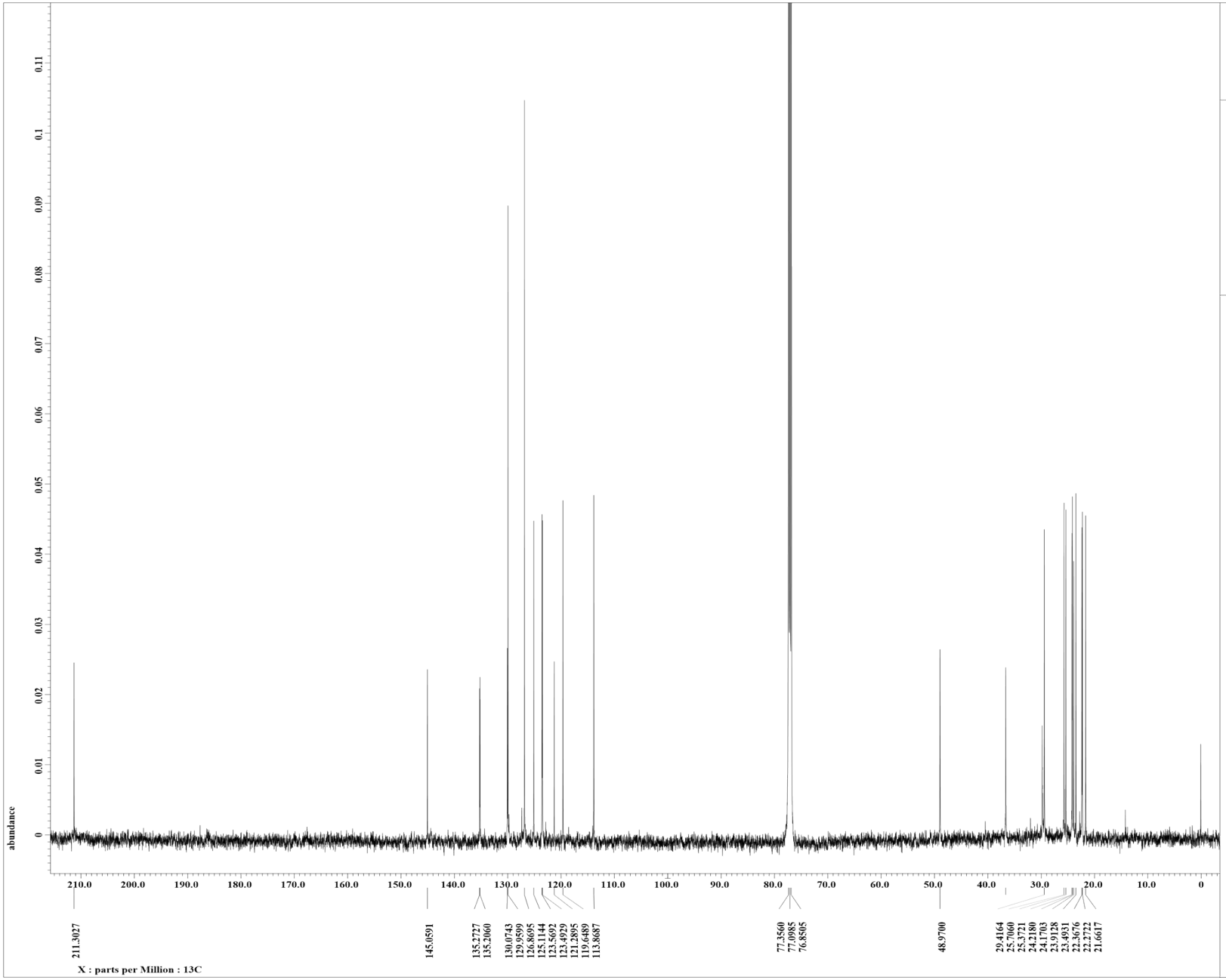






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA191007-2.jdf
```

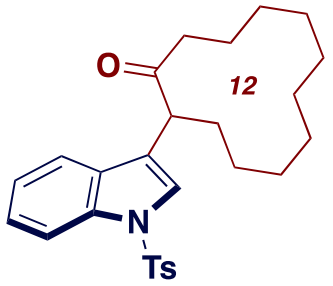
```
Filename          = TA191007-5.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#554909
Solvent           = CHLOROFORM-D
Creation_time     =  7-OCT-2019 14:49:48
Revision_time     =  8-MAY-2020 08:10:51
Current_time      =  8-MAY-2020 08:11:22

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 19.9[dC]
```

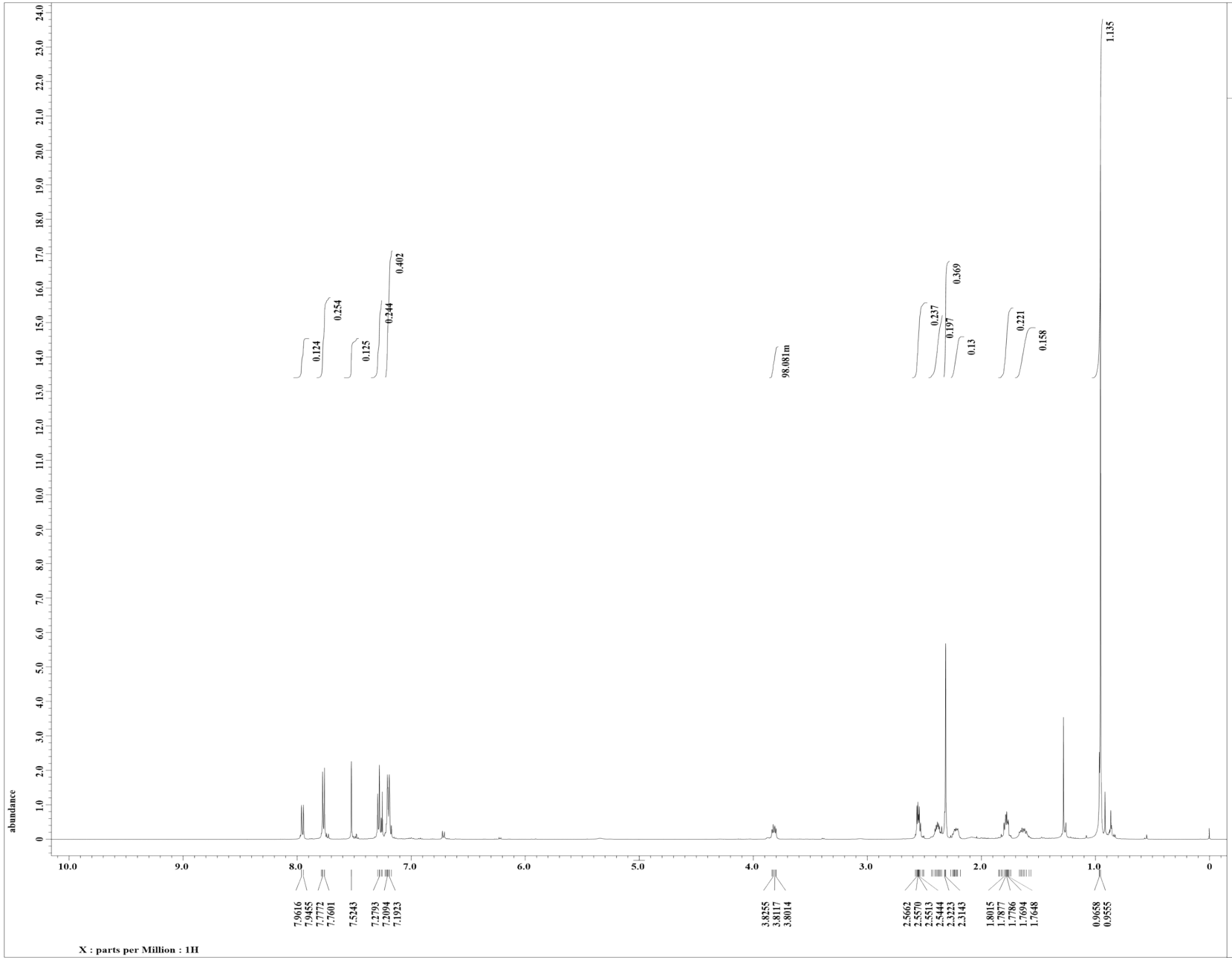


JEOL

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2019-1007-12-1.jdf
```

```
Filename          = TA2019-1007-12-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#620234
Solvent           = CHLOROFORM-D
Creation_time     =  8-OCT-2019 08:00:14
Revision_time     =  7-MAY-2020 13:09:15
Current_time      =  7-MAY-2020 13:10:16

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 18950
Total_scans       = 18950

X_90_width        = 12.8[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 5.3[dB]
X_pulse           = 4.26666667[us]
Irr_atn_dec       = 21.09[dB]
Irr_atn_noe       = 21.09[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 22.7[dC]
```



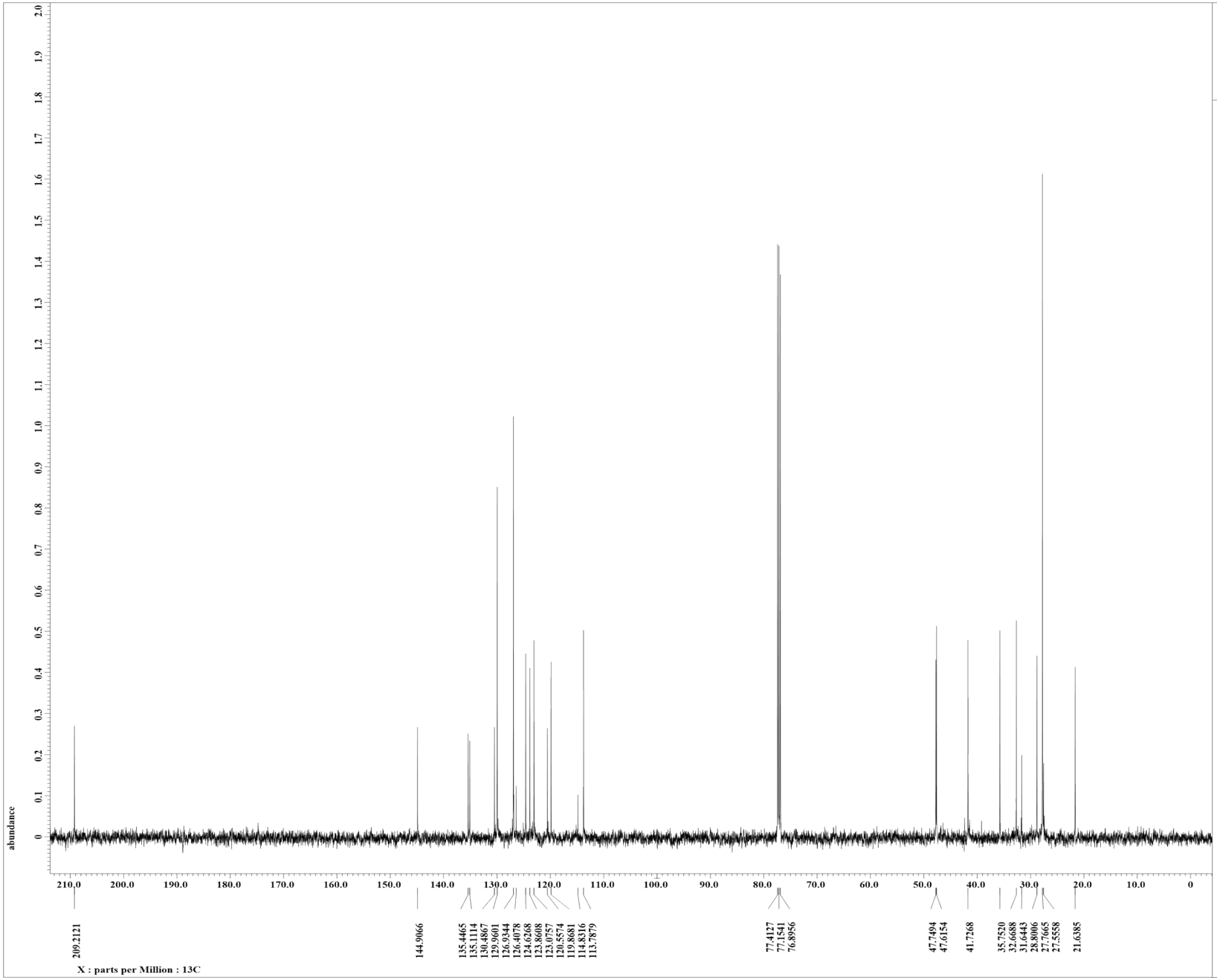


Filename = TA200618-4-tert-Bu-cy
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#592927
Solvent = CHLOROFORM-D
Creation_time = 18-JUN-2020 15:51:02
Revision_time = 18-JUN-2020 16:44:13
Current_time = 18-JUN-2020 16:45:11

Content = Fr20-25
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.3[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_pulse = 5.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 24.4[dC]

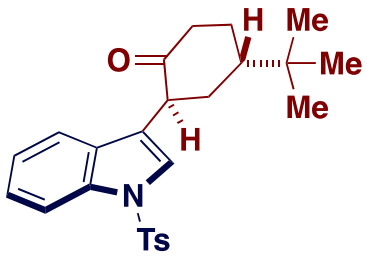


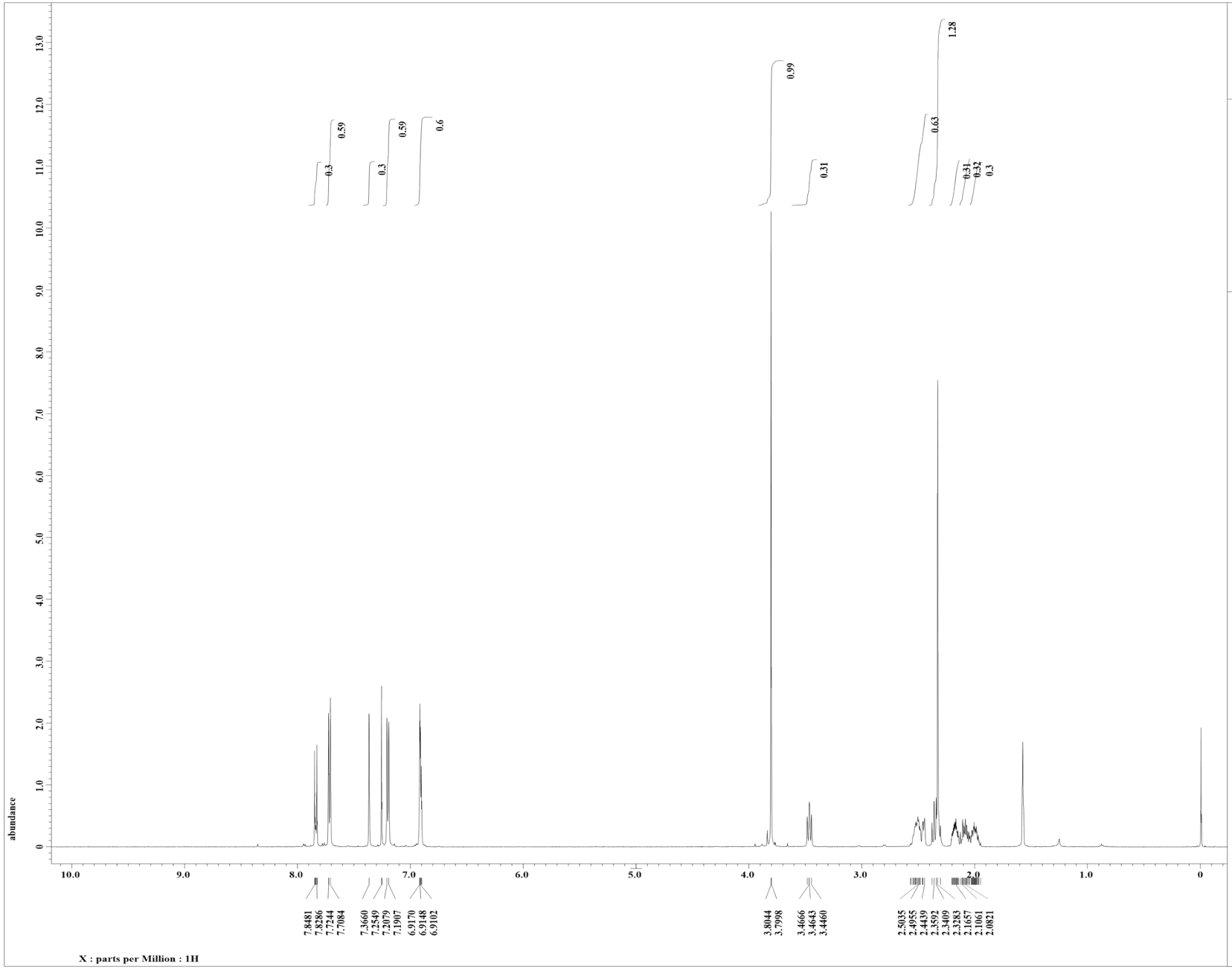
Filename = TA200618-4-tert-Bu-cy
Author = delta
Experiment = single_pulse_dec
Sample_id = S#600953
Solvent = CHLOROFORM-D
Creation_time = 18-JUN-2020 16:10:38
Revision_time = 19-JUN-2020 07:55:11
Current_time = 19-JUN-2020 07:55:42

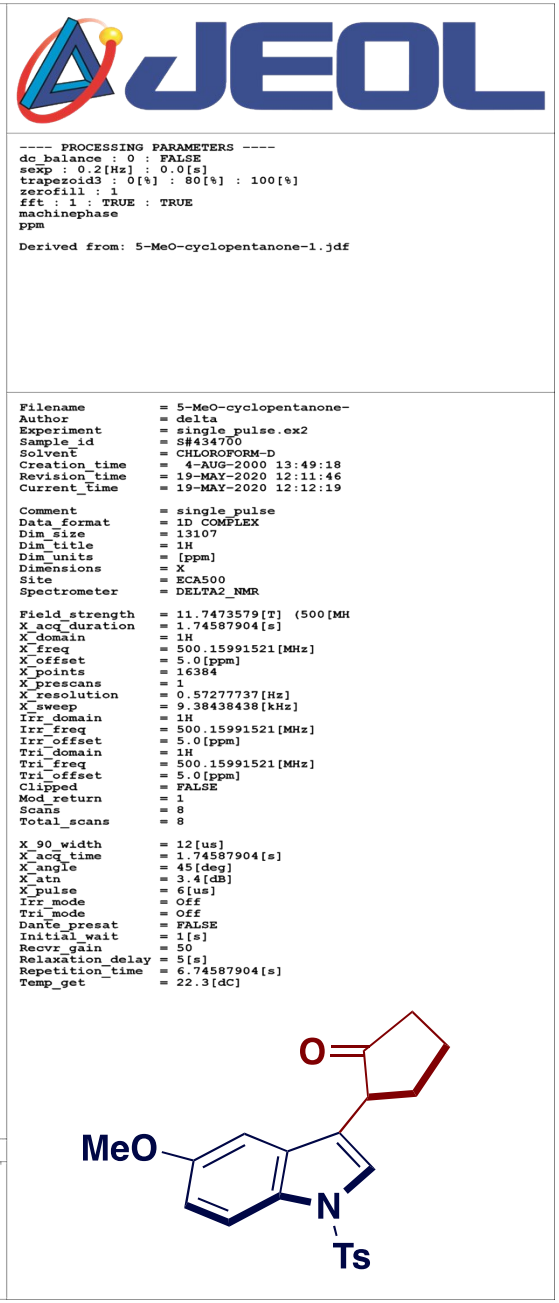
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Incomplete_copy = TRUE
Mod_return = 1
Scans = 144
Total_scans = 144

X_90_width = 10.1[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.36666667[us]
Irr_atn_dec = 21.51[dB]
Irr_atn_noe = 21.51[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get = 24.8[dC]

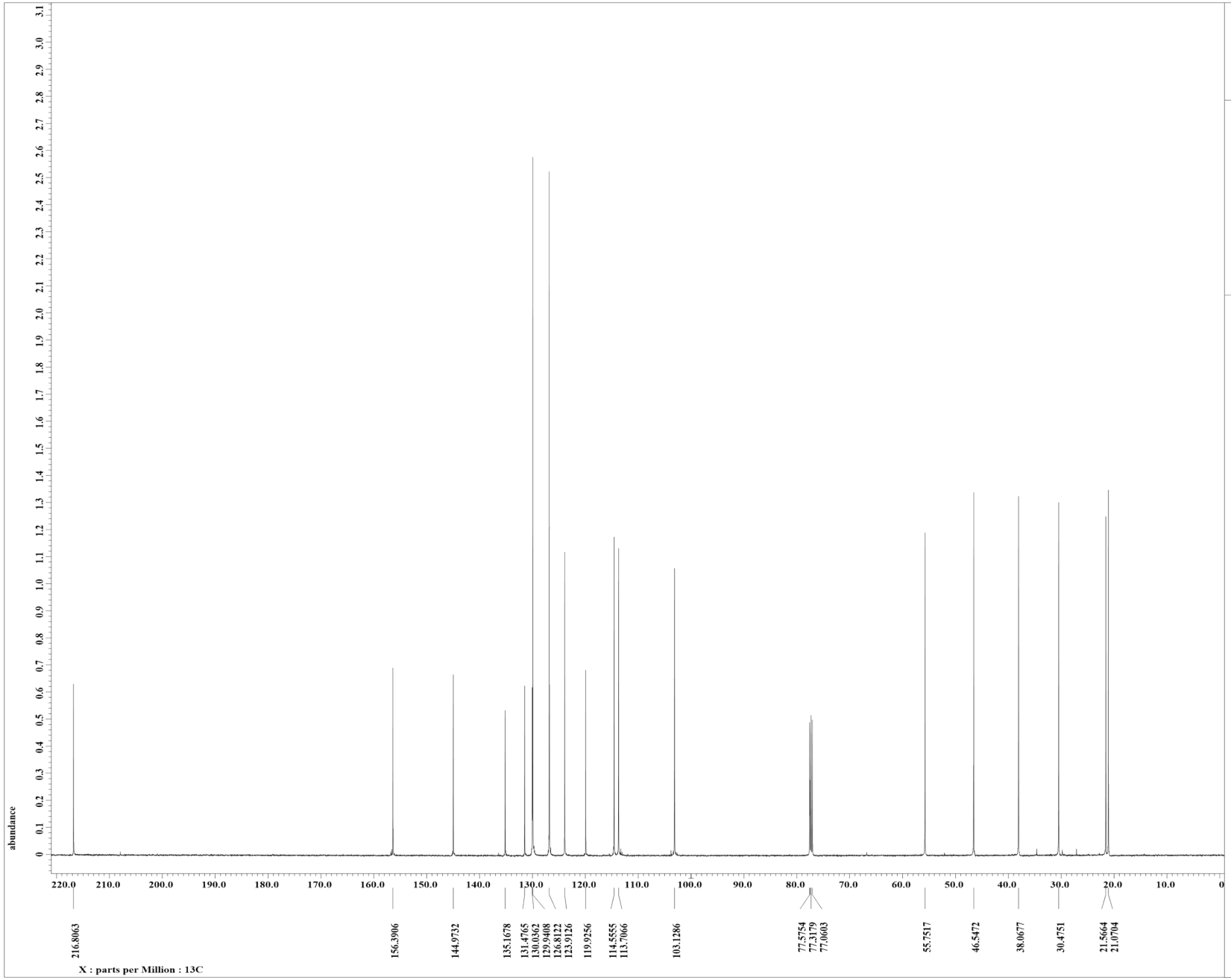


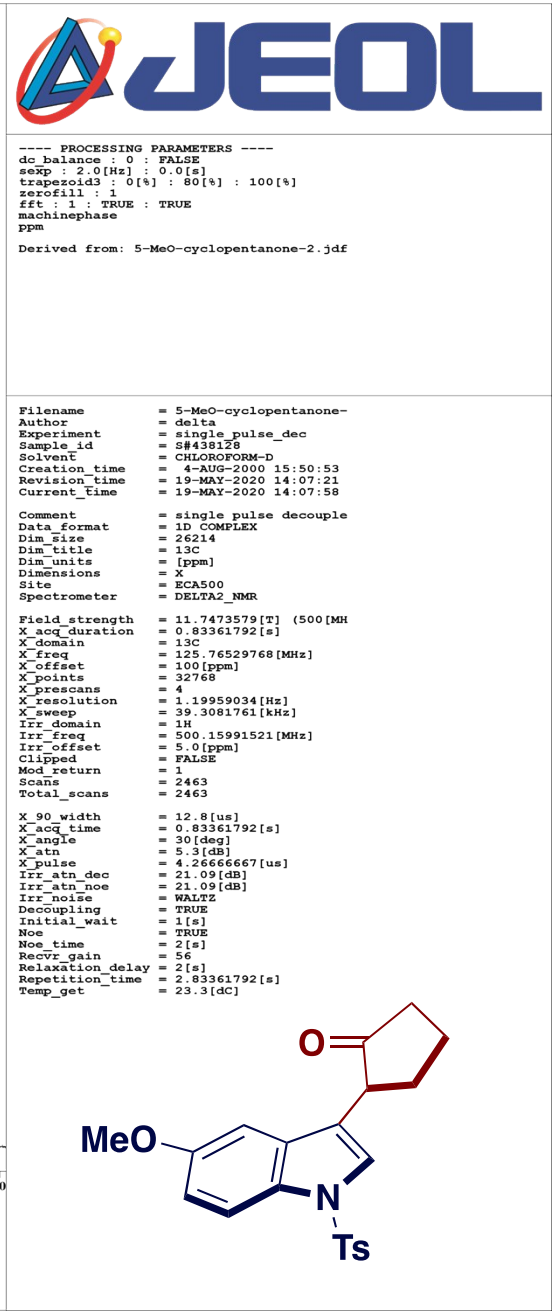




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 5-MeO-cyclopentanone-1.jdf
```

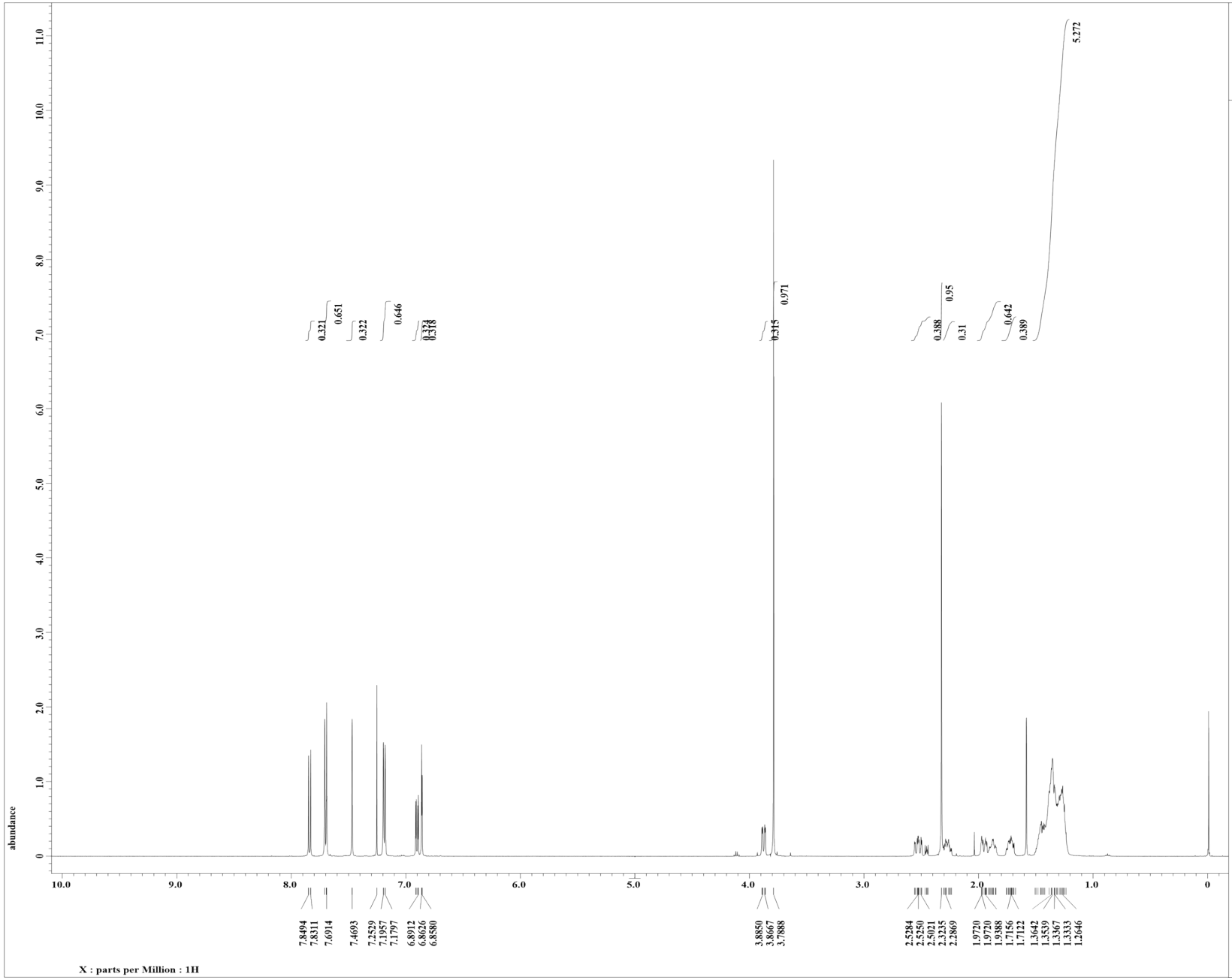
```
Filename          = 5-MeO-cyclopentanone-
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#434700
Solvent           = CHLOROFORM-D
Creation_time     =  4-AUG-2000 13:49:18
Revision_time     = 19-MAY-2020 12:11:46
Current_time      = 19-MAY-2020 12:12:19

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 6[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.74587904[s]
Temp_get          = 22.3[dC]
```

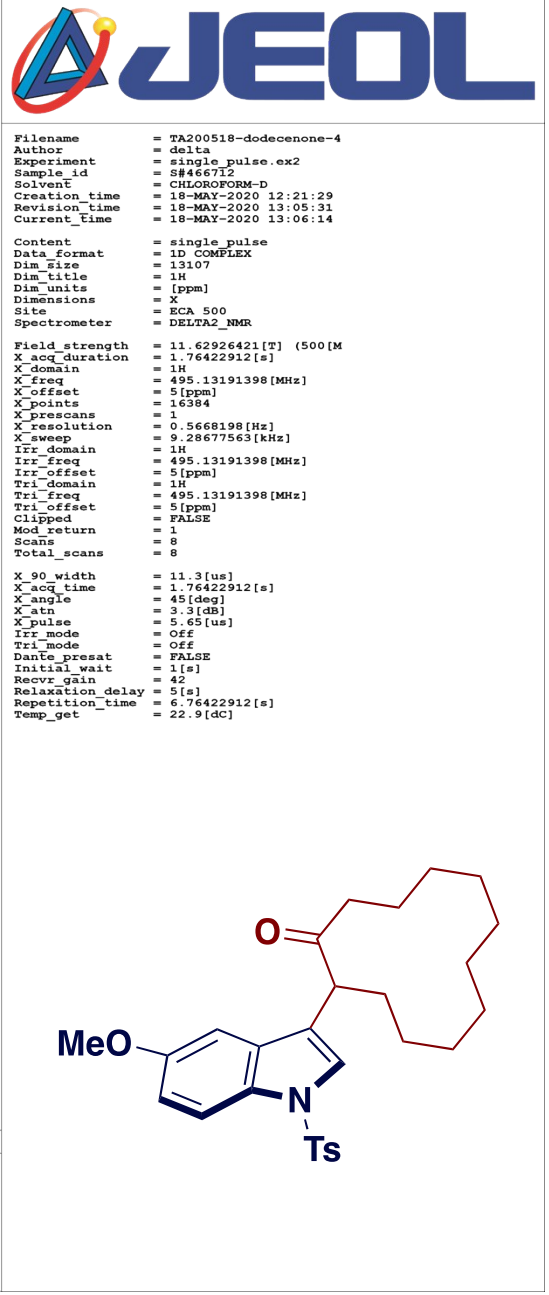




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 5-MeO-cyclopentanone-2.jdf
```

Filename	= 5-MeO-cyclopentanone-
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#438128
Solvent	= CHLOROFORM-D
Creation_time	= 4-AUG-2000 15:50:53
Revision_time	= 19-MAY-2020 14:07:21
Current_time	= 19-MAY-2020 14:07:58
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 2463
Total_scans	= 2463
X_90_width	= 12.8[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 5.3[dB]
X_pulse	= 4.26666667[us]
Irr_atn_dec	= 21.09[dB]
Irr_atn_noe	= 21.09[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 56
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23.3[dC]



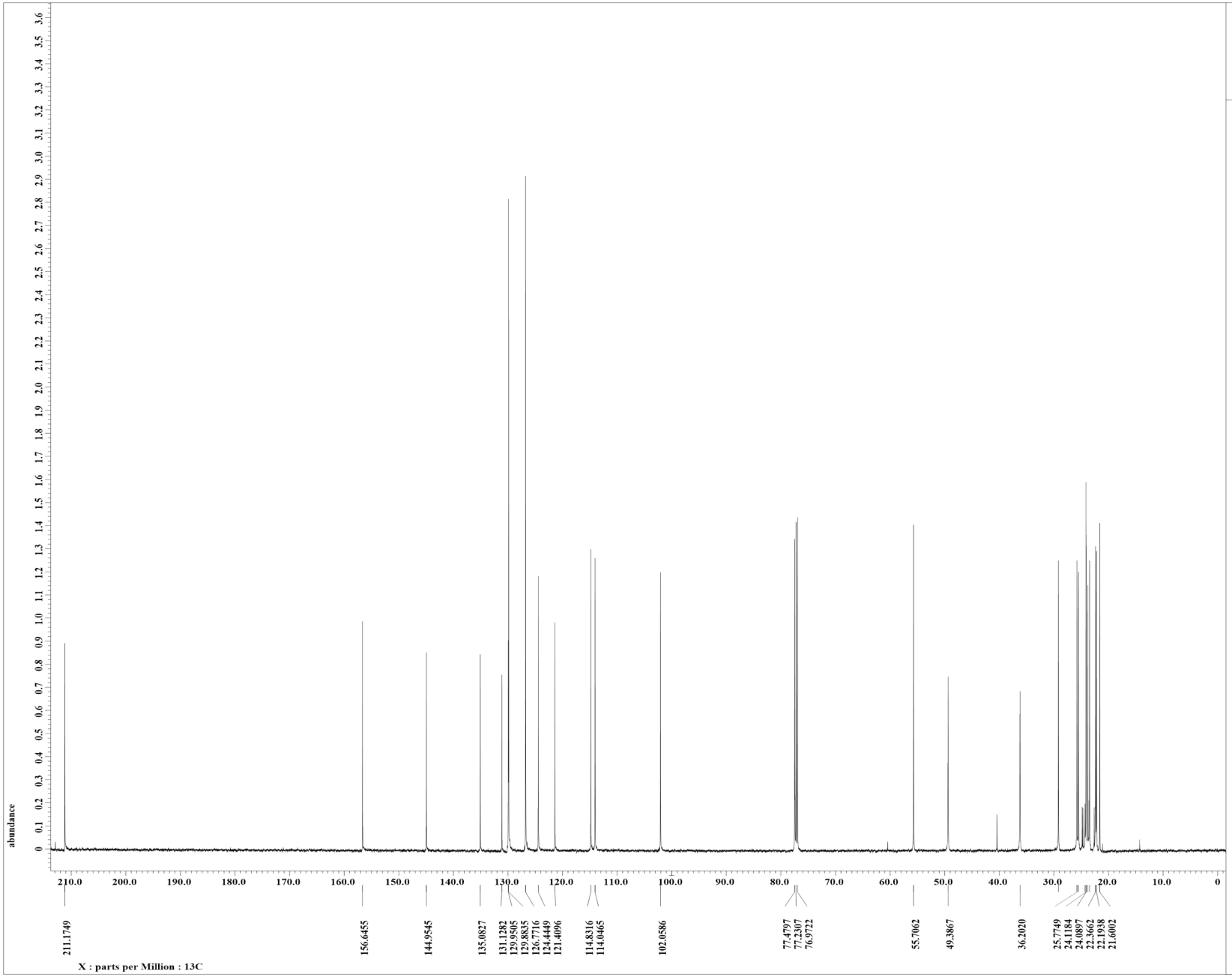


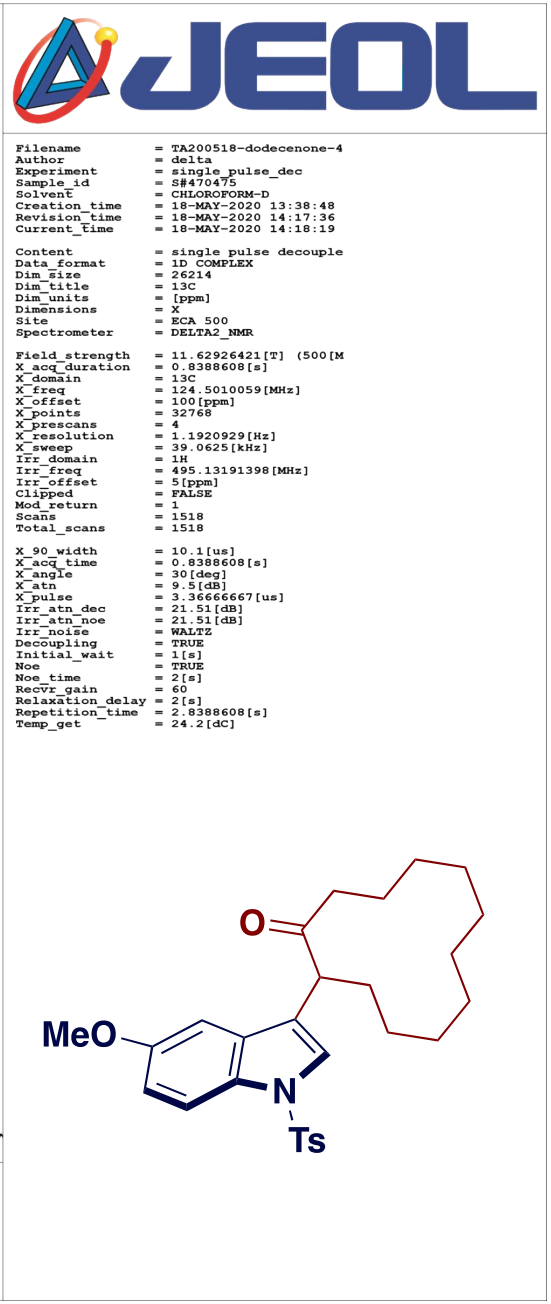
Filename = TA200518-dodecenone-4
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#4667I2
Solvent = CHLOROFORM-D
Creation_time = 18-MAY-2020 12:21:29
Revision_time = 18-MAY-2020 13:05:31
Current_time = 18-MAY-2020 13:06:14

Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

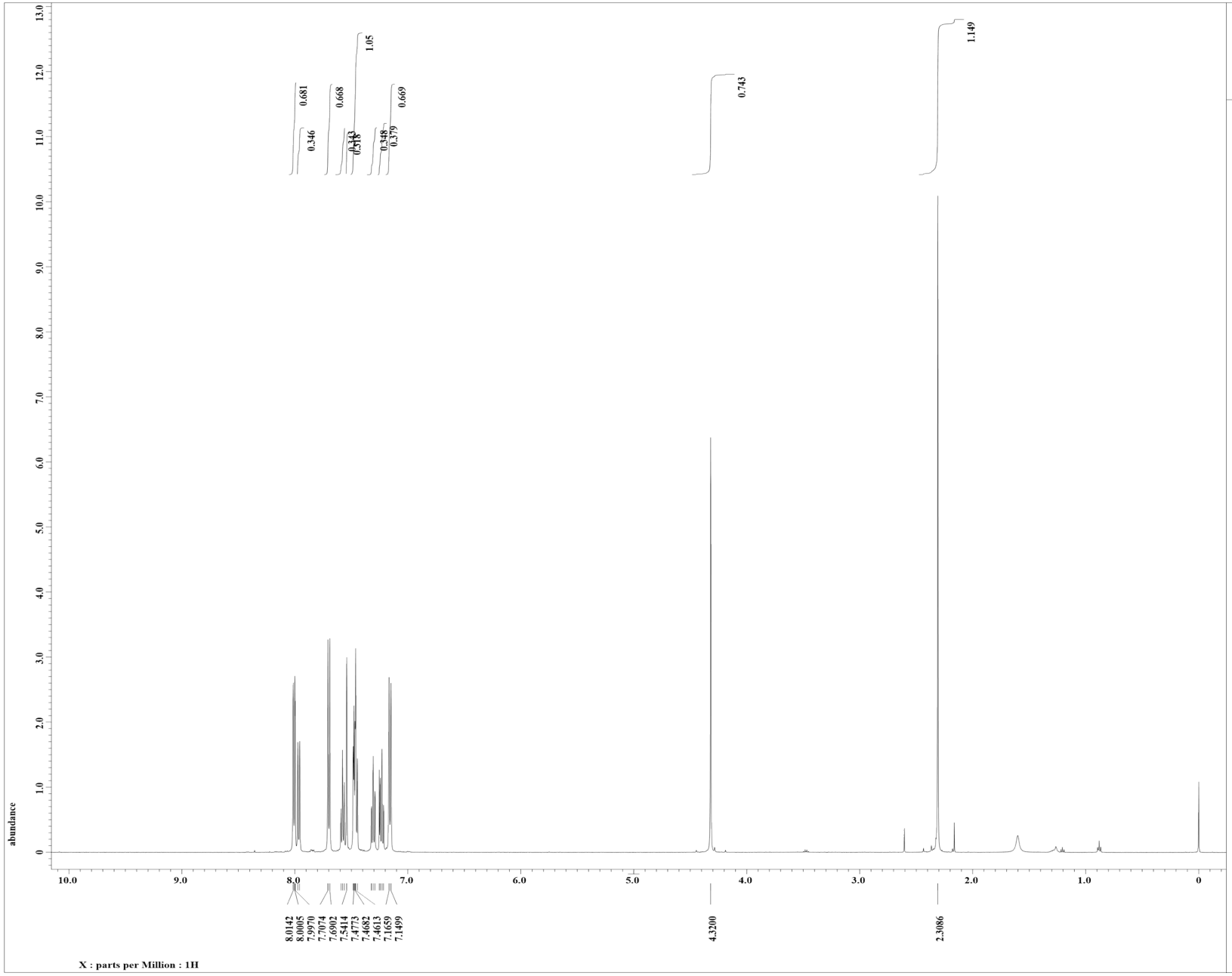
Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.3[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_pulse = 5.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 22.9[dC]



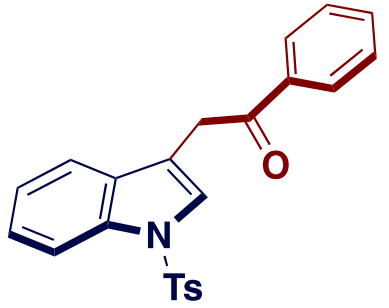


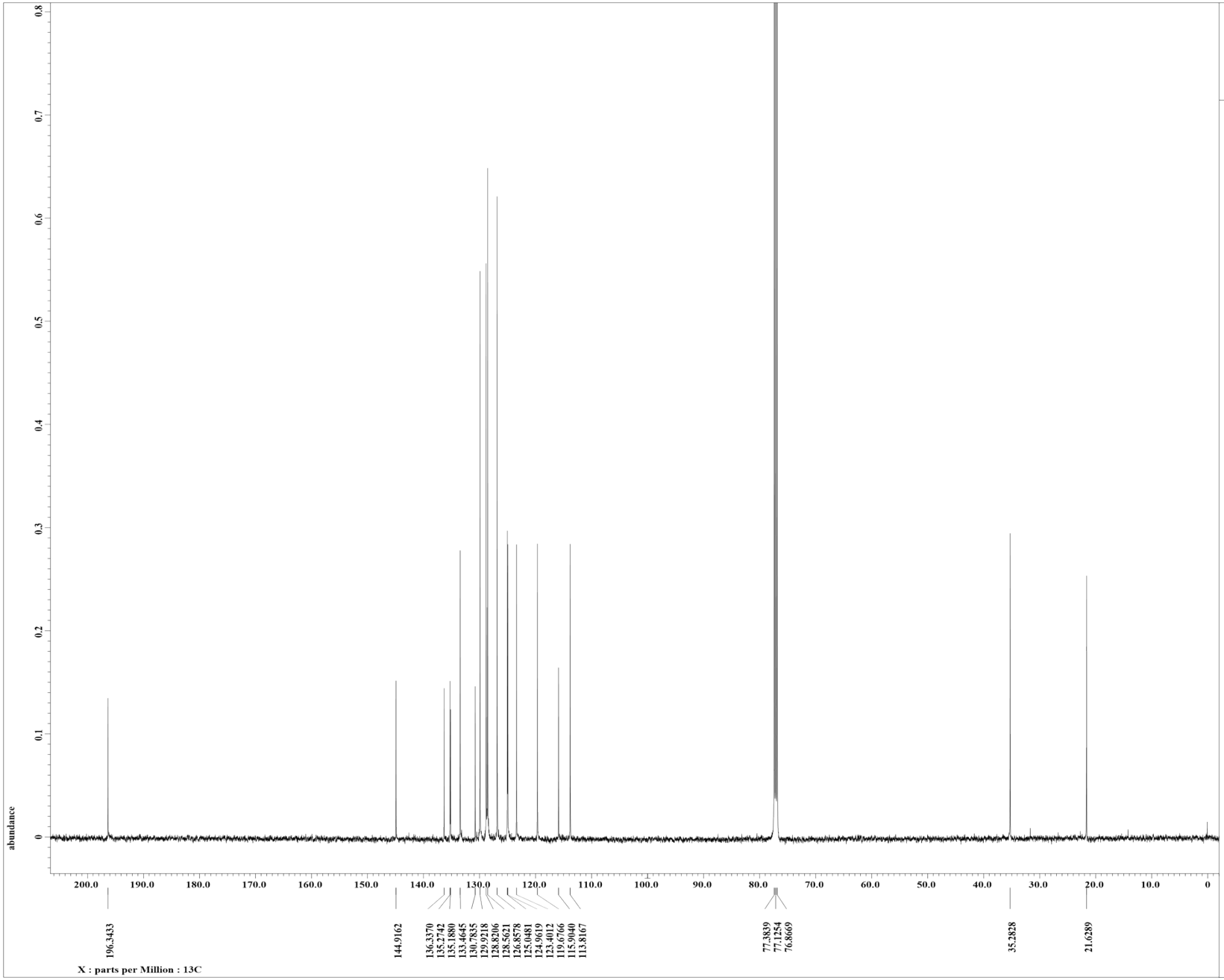
```
Filename          = TA200518-dodecenone-4
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#470475
Solvent           = CHLOROFORM-D
Creation_time     = 18-MAY-2020 13:38:48
Revision_time     = 18-MAY-2020 14:17:36
Current_time      = 18-MAY-2020 14:18:19

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1518
Total_scans       = 1518

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 24.2[dC]
```



JEOL

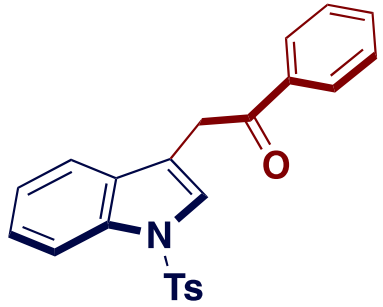
```
Filename          = TA200529-acetophenone
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#479939
Solvent           = CHLOROFORM-D
Creation_time     = 29-MAY-2020 12:41:47
Revision_time     = 29-MAY-2020 13:24:21
Current_time      = 29-MAY-2020 13:24:52

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 24[dC]
```

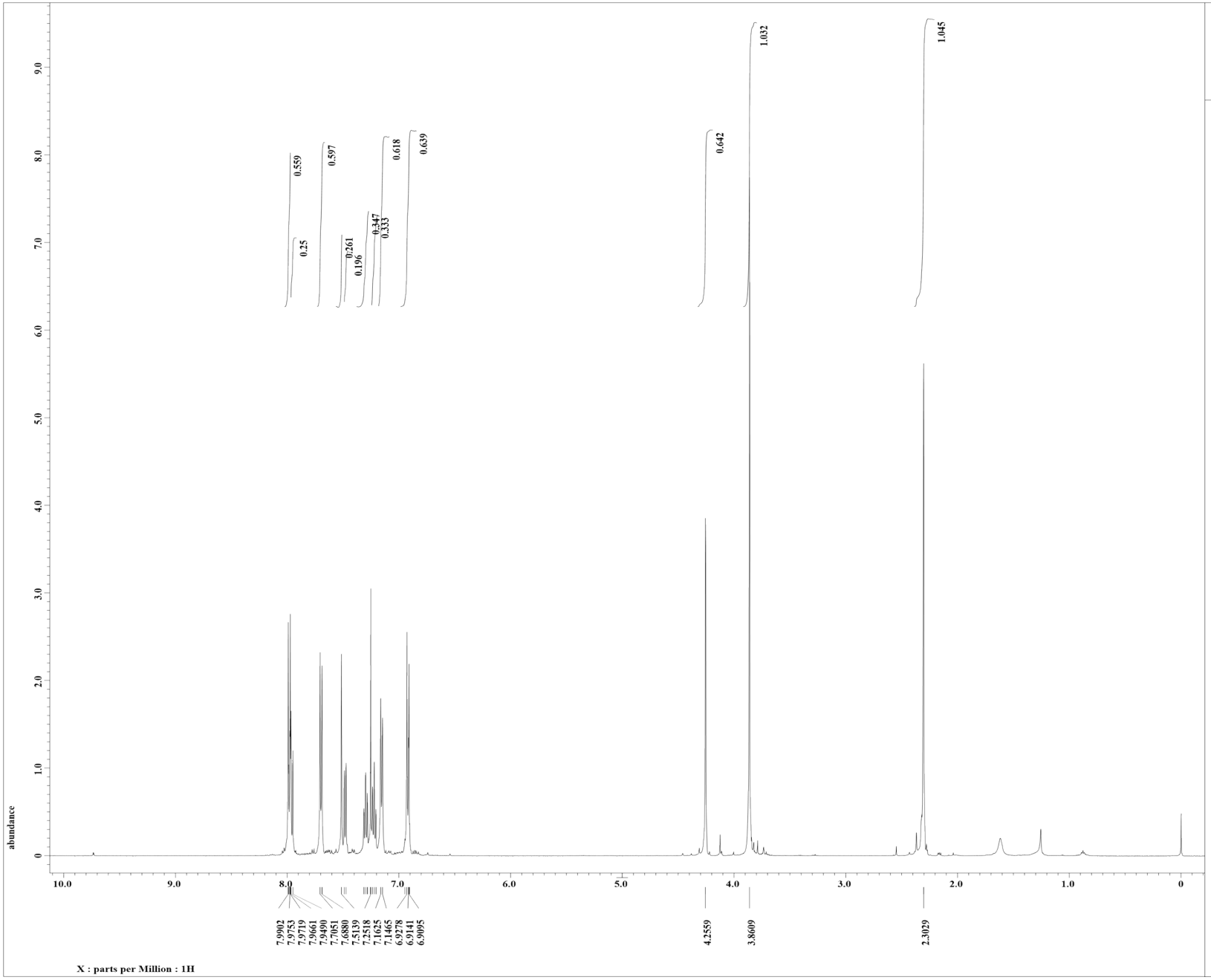




JEOL

```
Filename          = TA200529-acetophenone
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#4813I3
Solvent           = CHLOROFORM-D
Creation_time     = 29-MAY-2020 16:53:55
Revision_time     = 29-MAY-2020 17:35:45
Current_time      = 29-MAY-2020 17:36:14

Content           = Ts-acetophenone-2
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 5297
Total_scans       = 5297

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
RecVr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 25[dC]
```



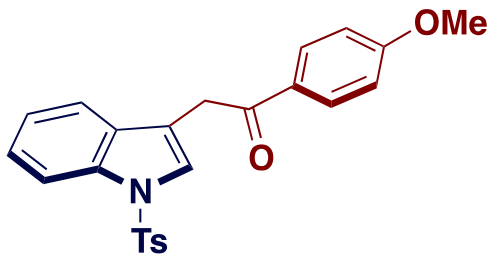


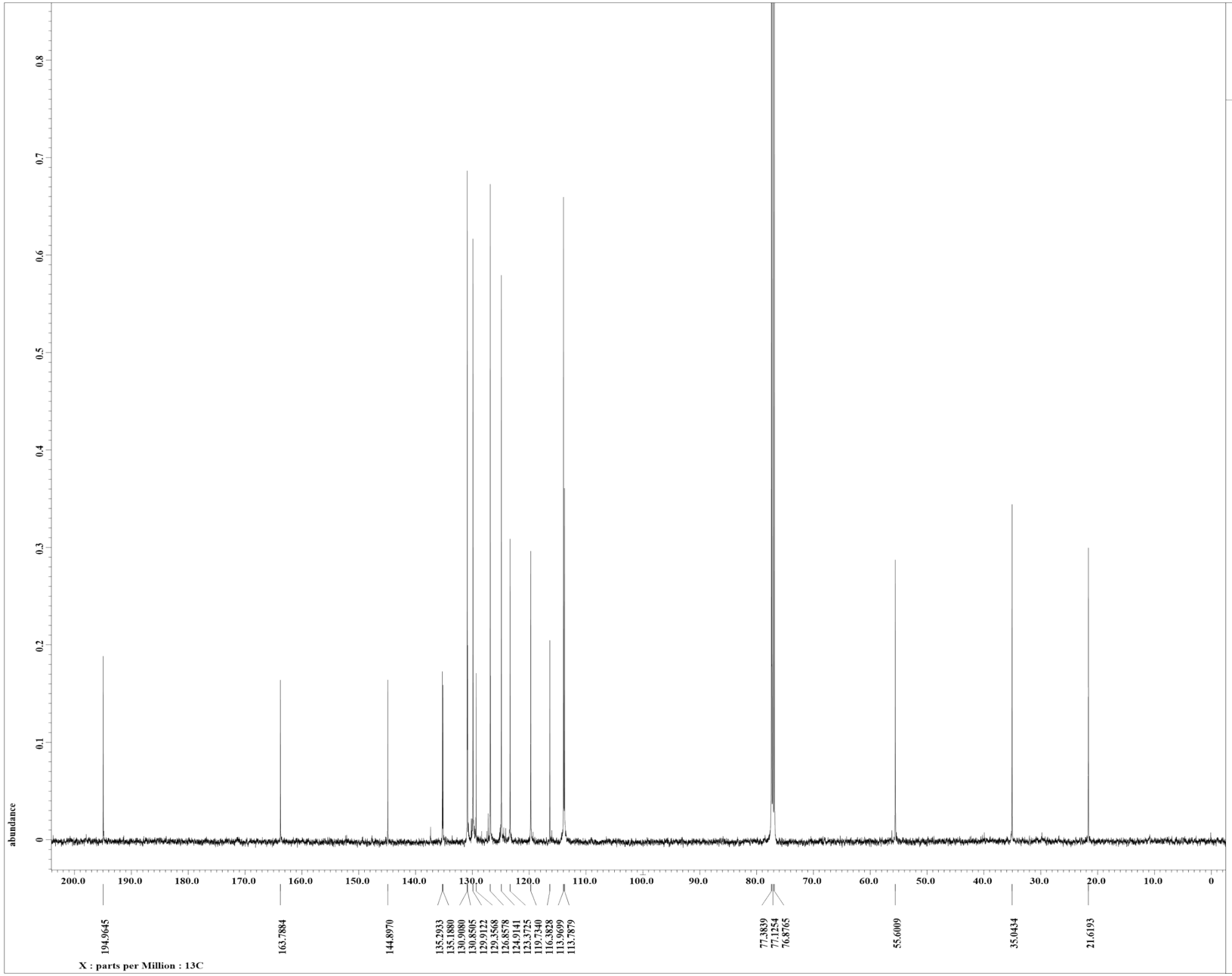
Filename = Ta200603-5H-4-MeO-ace
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#297984
Solvent = CHLOROFORM-D
Creation_time = 3-JUN-2020 07:37:48
Revision_time = 3-JUN-2020 08:23:33
Current_time = 3-JUN-2020 08:24:26

Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

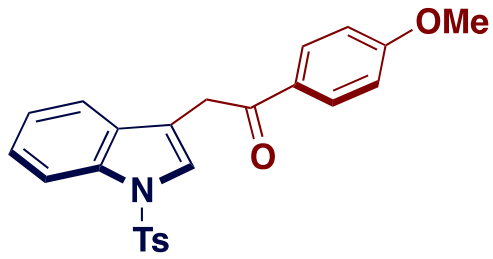
Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

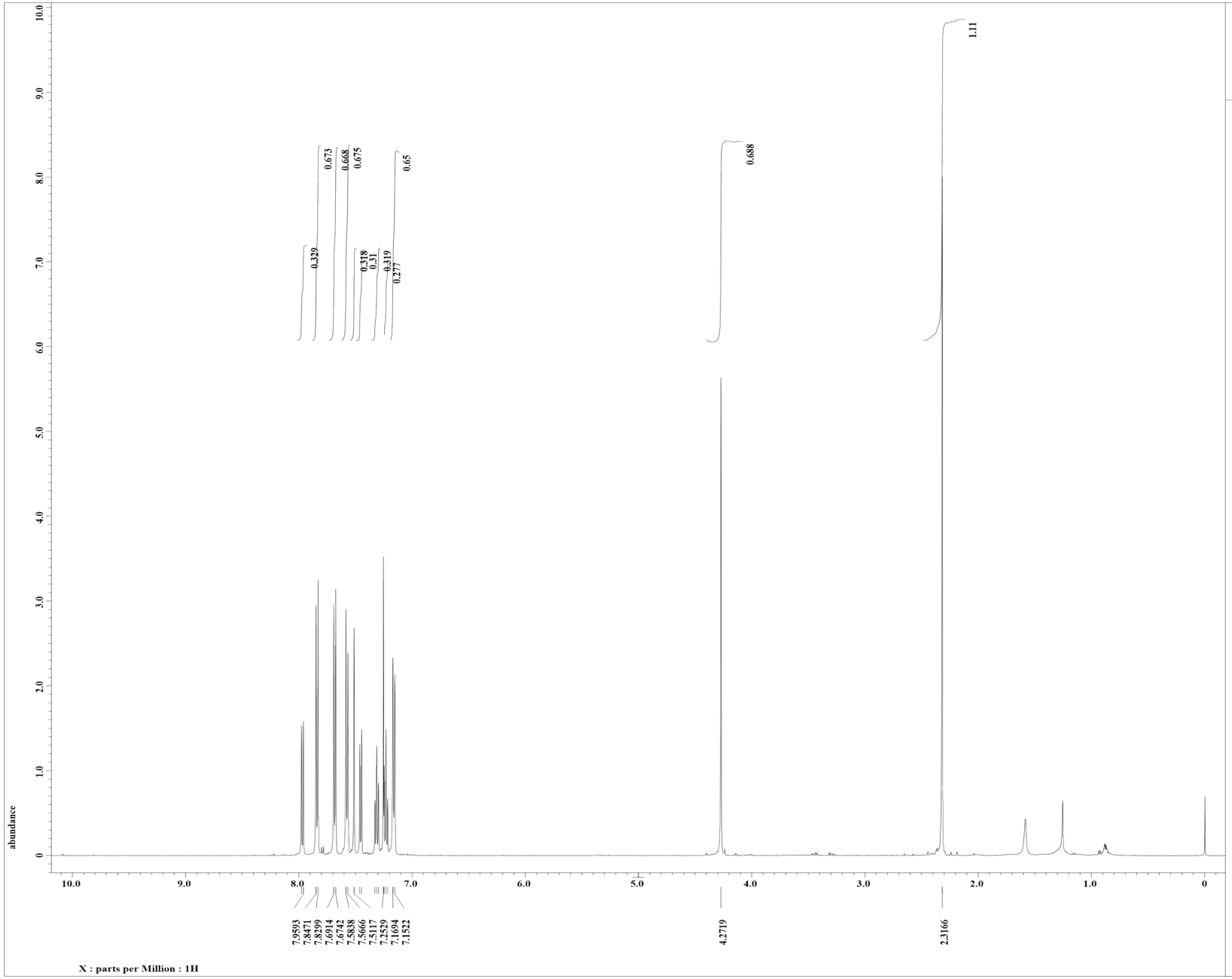
X_90_width = 11.3[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_pulse = 5.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 24.7[dC]





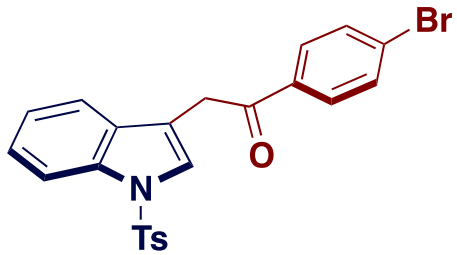

```
Filename          = Ta200603-5H-4-MeO-ace
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#607425
Solvent           = CHLOROFORM-D
Creation_time     =  3-JUN-2020 18:50:13
Revision_time     =  3-JUN-2020 19:33:21
Current_time      =  3-JUN-2020 19:33:58

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 3329
Total_scans       = 3329

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 25.2[dC]
```

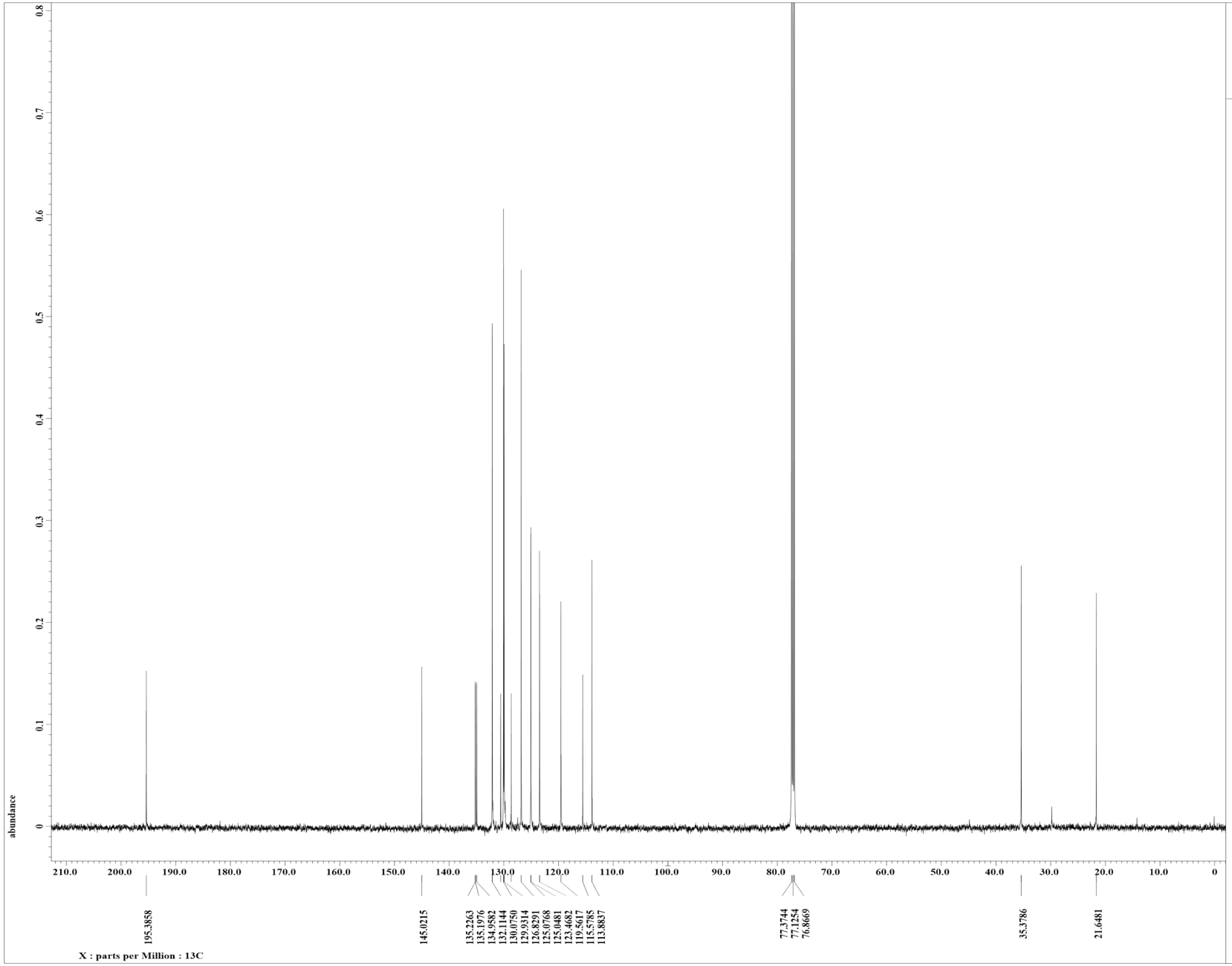




JEOL

```
Filename          = Ta200603-5H-4_Br-acet
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#307584
Solvent           = CHLOROFORM-D
Creation_time     =  4-JUN-2020 07:53:38
Revision_time     =  4-JUN-2020 08:36:51
Current_time      =  4-JUN-2020 08:37:20

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 24.5[dC]
```



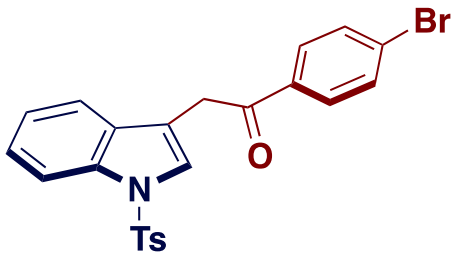


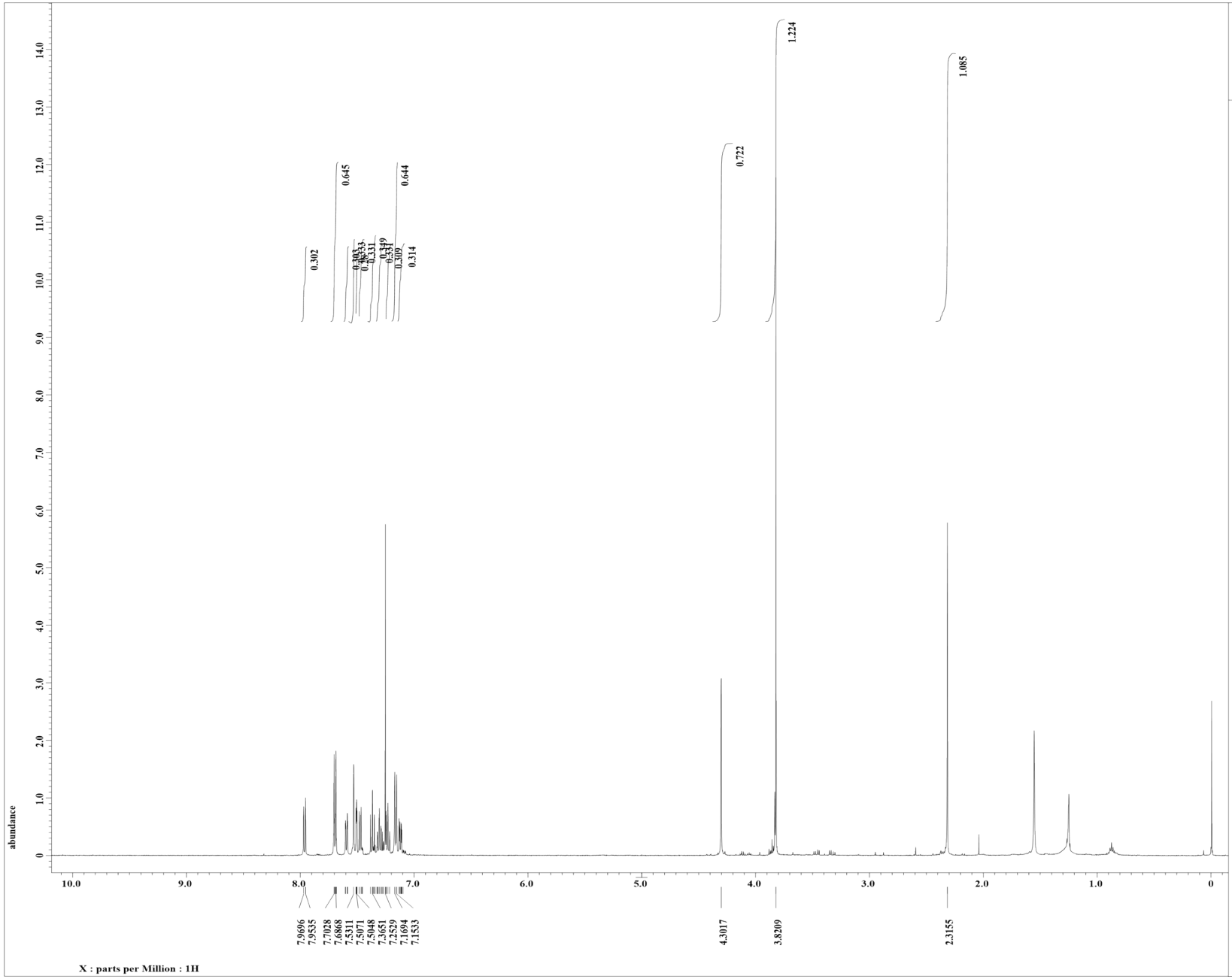
Filename = Ta200603-5H-4_Br-acet
Author = delta
Experiment = single_pulse_dec
Sample_id = S#311755
Solvent = CHLOROFORM-D
Creation_time = 4-JUN-2020 11:09:32
Revision_time = 4-JUN-2020 11:51:05
Current_time = 4-JUN-2020 11:51:53

Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4010
Total_scans = 4010

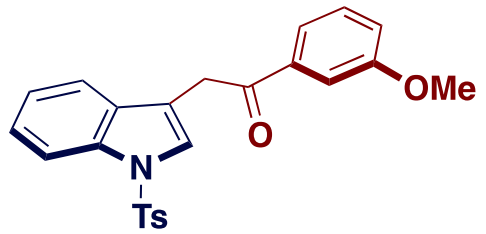
X_90_width = 10.1[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.36666667[us]
Irr_atn_dec = 21.51[dB]
Irr_atn_noe = 21.51[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get = 25[dC]

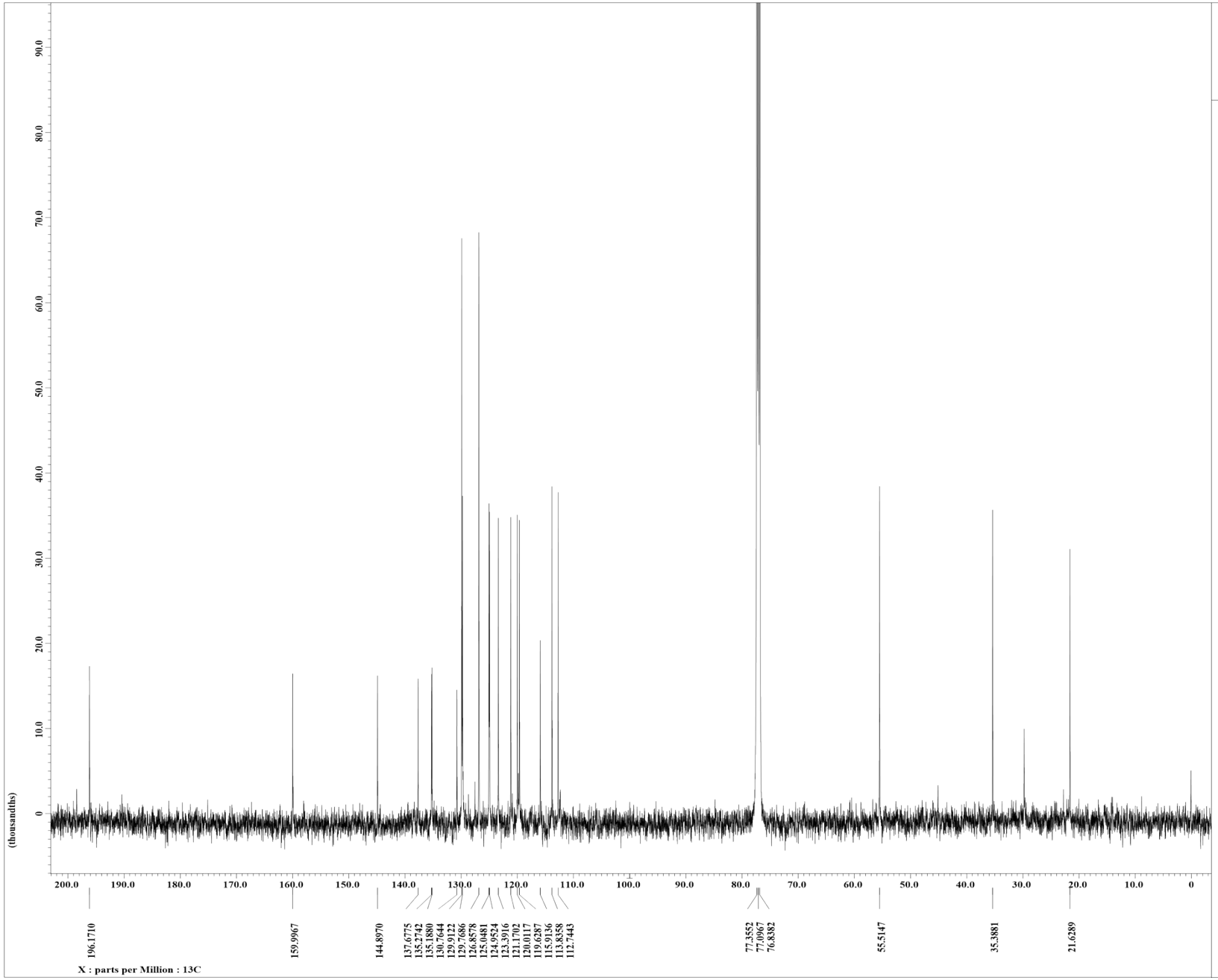




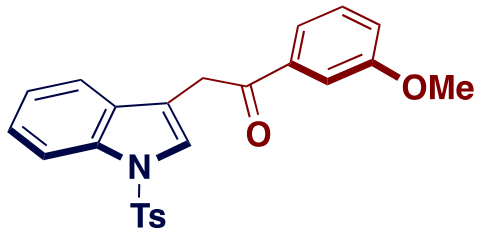
JEOL

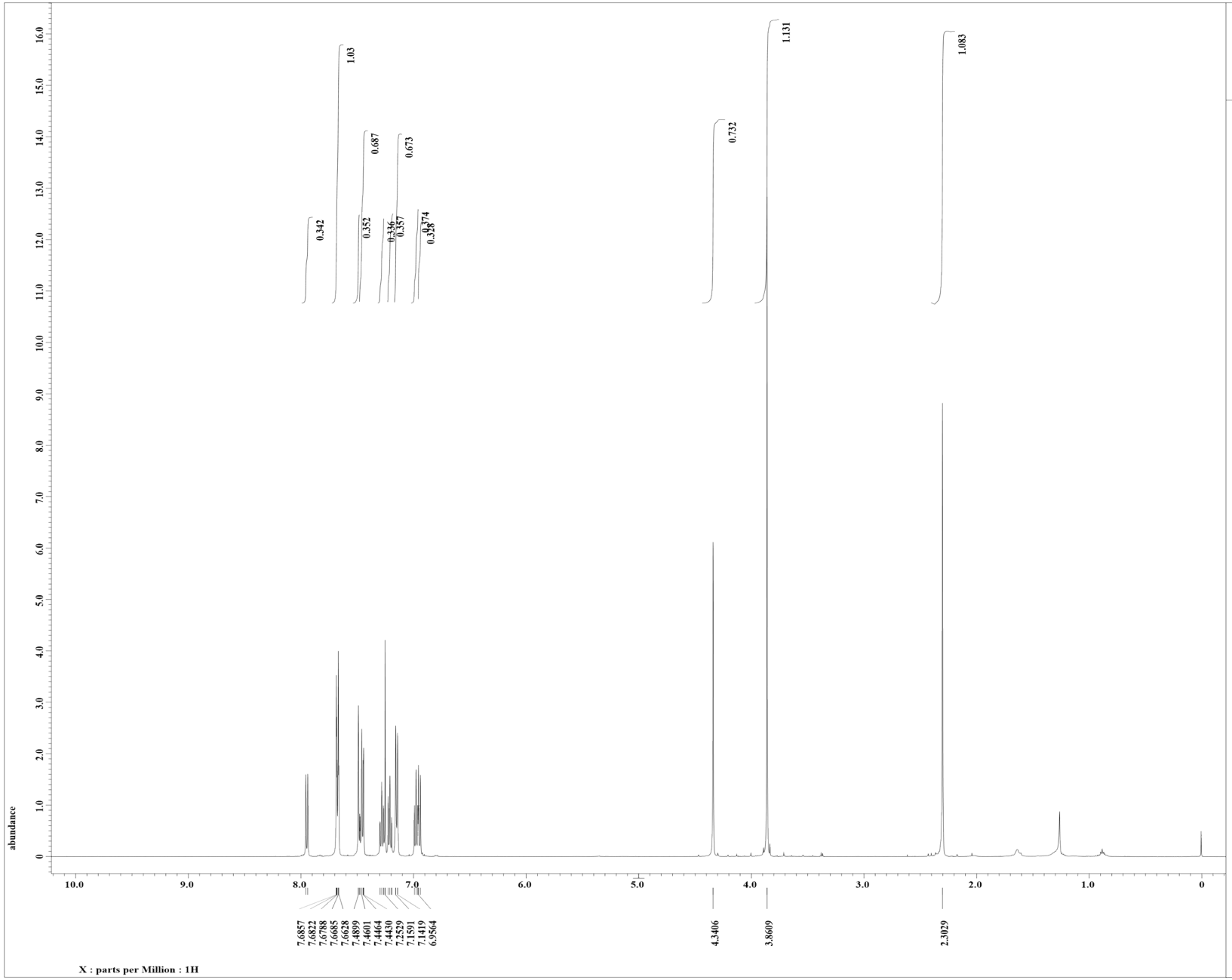
```
Filename          = 5H-3MeO-acetophenone-
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#715472
Solvent           = CHLOROFORM-D
Creation_time     = 10-JUN-2020 19:11:55
Revision_time     = 11-JUN-2020 08:04:53
Current_time      = 11-JUN-2020 08:05:24

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 24.4[dC]
```





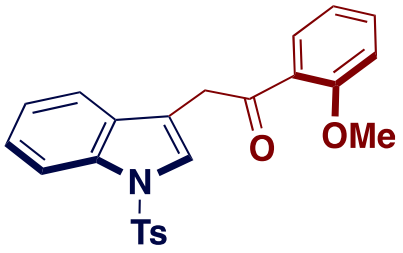
```
Filename          = 5H-3MeO-acetophenone-
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#716537
Solvent           = CHLOROFORM-D
Creation_time     = 11-JUN-2020 07:29:27
Revision_time     = 11-JUN-2020 08:07:45
Current_time      = 11-JUN-2020 08:08:38

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 15556
Total_scans       = 15556

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
RecVr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 25.1[dC]
```

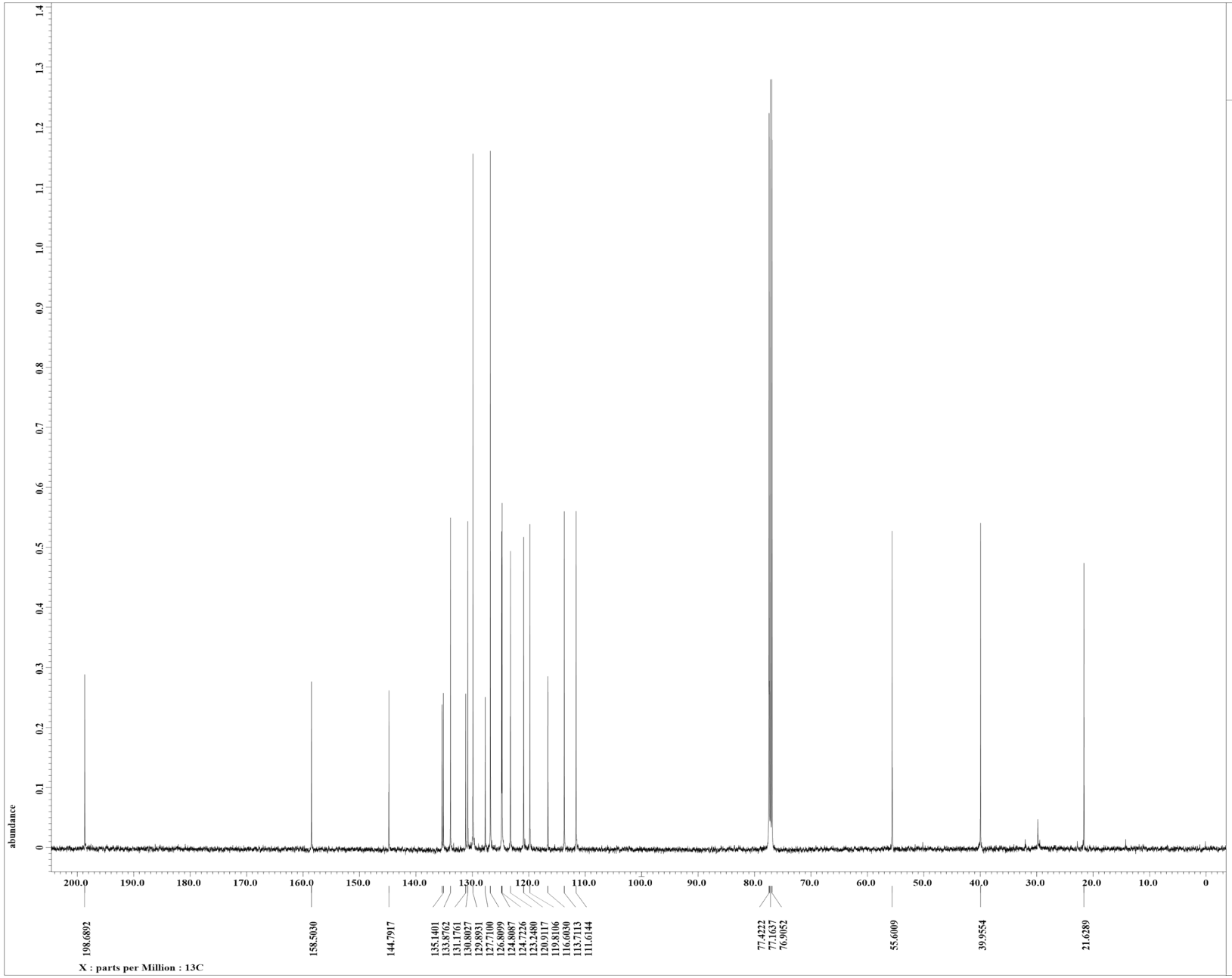




JEOL

```
Filename          = 5H-2MeO-acetophenone-
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#532652
Solvent           = CHLOROFORM-D
Creation_time     = 10-JUN-2020 14:07:43
Revision_time     = 10-JUN-2020 14:52:58
Current_time      = 10-JUN-2020 14:53:24

Content           = 1H-2MeOacetophenone
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 24.1[dC]
```



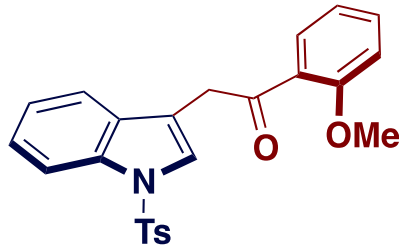


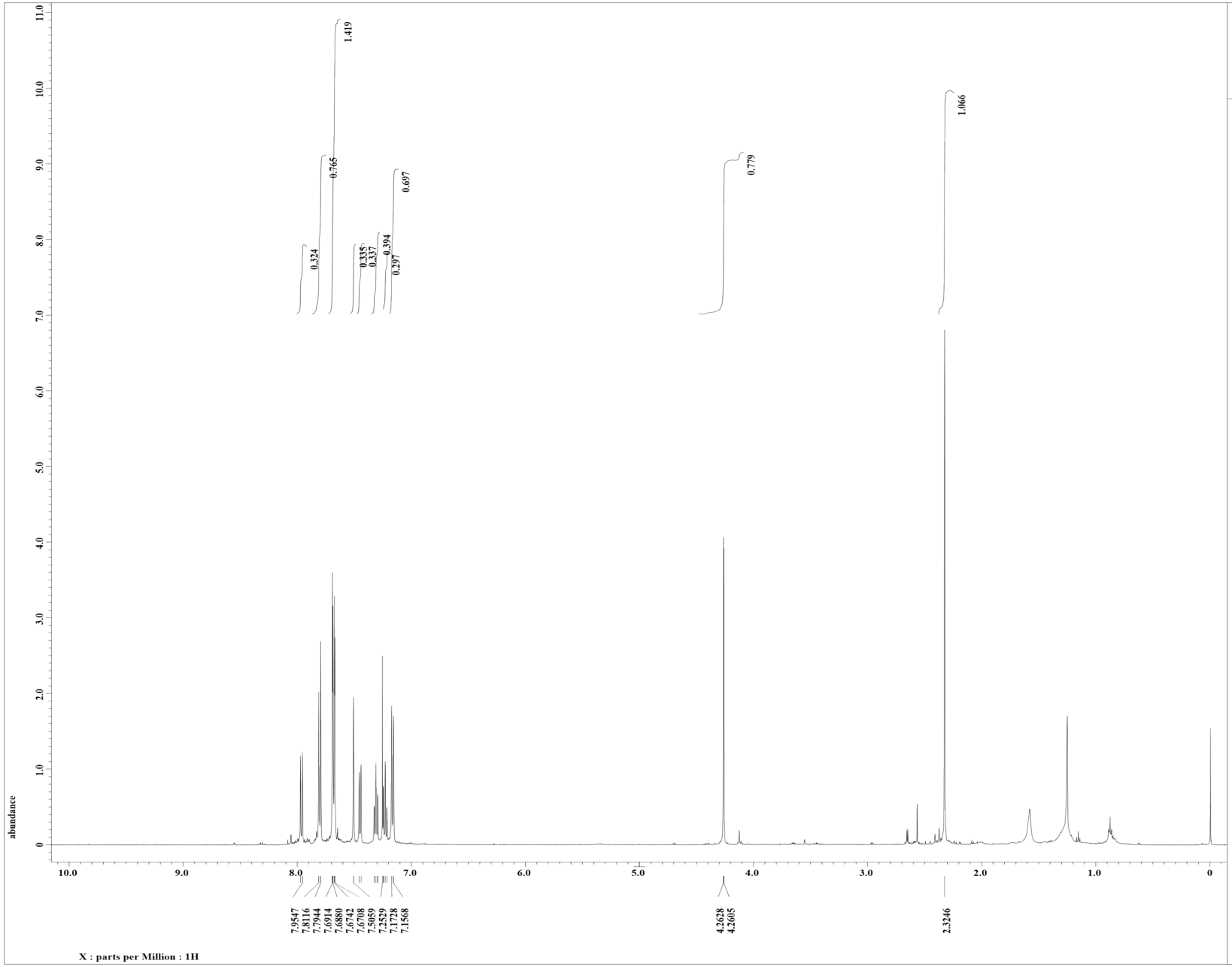
Filename = 5H-2MeO-acetophenone-
Author = delta
Experiment = single_pulse_dec
Sample_id = S#534021
Solvent = CHLOROFORM-D
Creation_time = 10-JUN-2020 15:49:55
Revision_time = 10-JUN-2020 16:32:15
Current_time = 10-JUN-2020 16:33:05

Content = 13C-2MeOacetophenone
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 2123
Total_scans = 2123

X_90_width = 10.1[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.36666667[us]
Irr_atn_dec = 21.51[dB]
Irr_atn_noe = 21.51[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
RecVr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get = 25[dC]



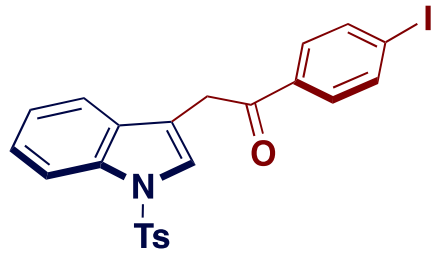


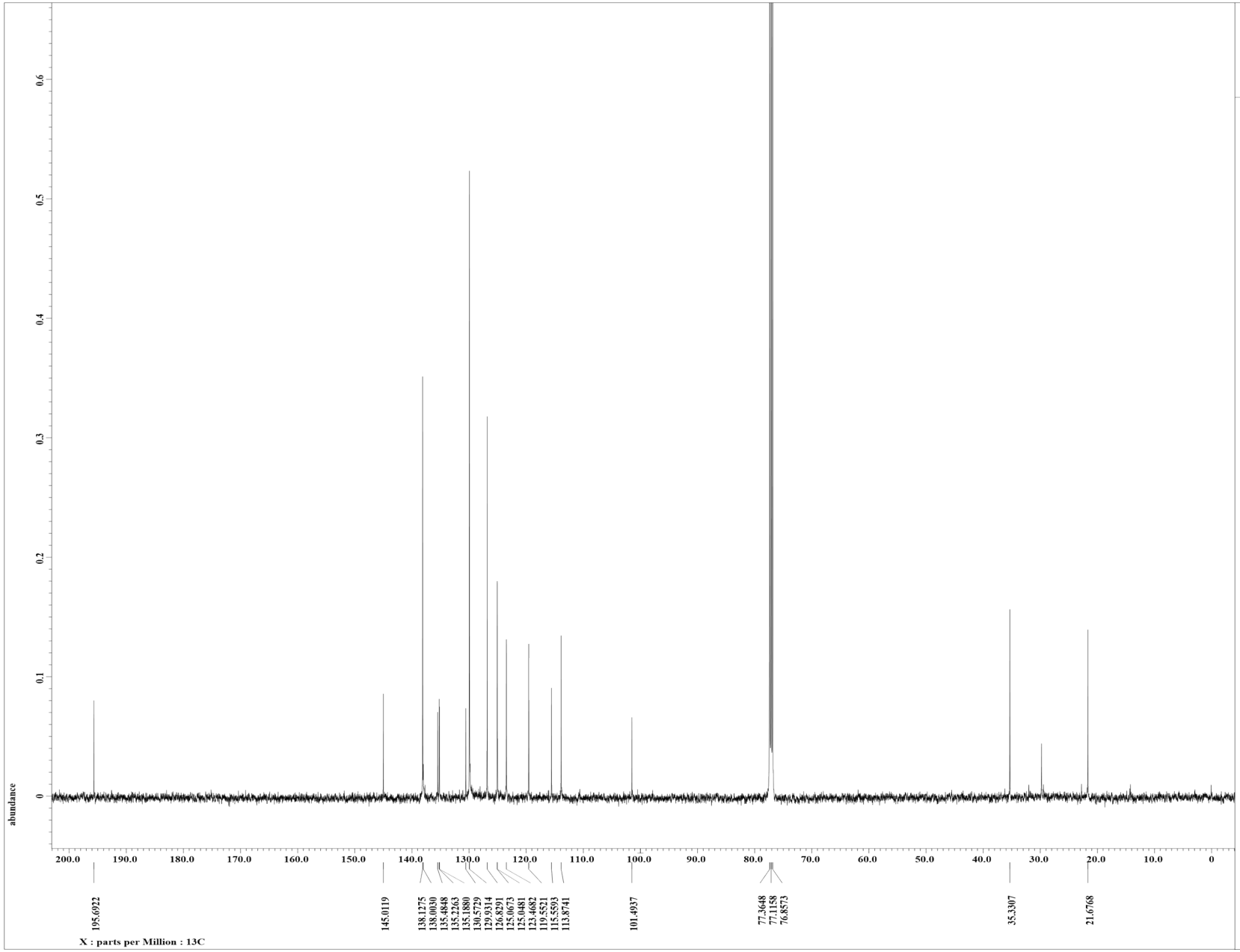
Filename = TA200617-4I-acetophen
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#339946
Solvent = CHLOROFORM-D
Creation_time = 17-JUN-2020 08:49:47
Revision_time = 17-JUN-2020 09:32:03
Current_time = 17-JUN-2020 09:32:58

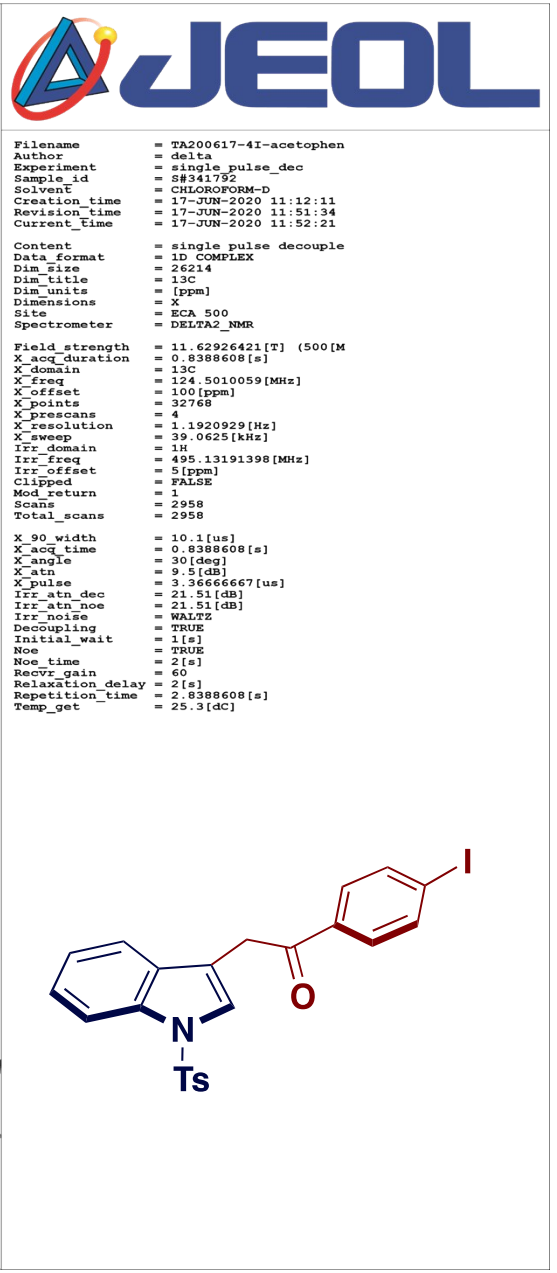
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.3[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_pulse = 5.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 24.5[dC]




abundance
0.6
0.5
0.4
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
195.6922
145.0119
138.1275
138.0030
135.4848
135.2263
135.1880
130.5729
129.9314
126.8291
125.0673
125.0481
123.4682
119.5521
115.5593
113.8741
101.4937
77.3648
77.1158
76.8573
35.3307
21.6768
X : parts per Million : 13C


Filename = TA200617-4I-acetophen
Author = delta
Experiment = single_pulse_dec
Sample_id = S#341792
Solvent = CHLOROFORM-D
Creation_time = 17-JUN-2020 11:12:11
Revision_time = 17-JUN-2020 11:51:34
Current_time = 17-JUN-2020 11:52:21
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR
Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 2958
Total_scans = 2958
X_90_width = 10.1[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.36666667[us]
Irr_atn_dec = 21.51[dB]
Irr_atn_noe = 21.51[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get = 25.3[dC]
I
O
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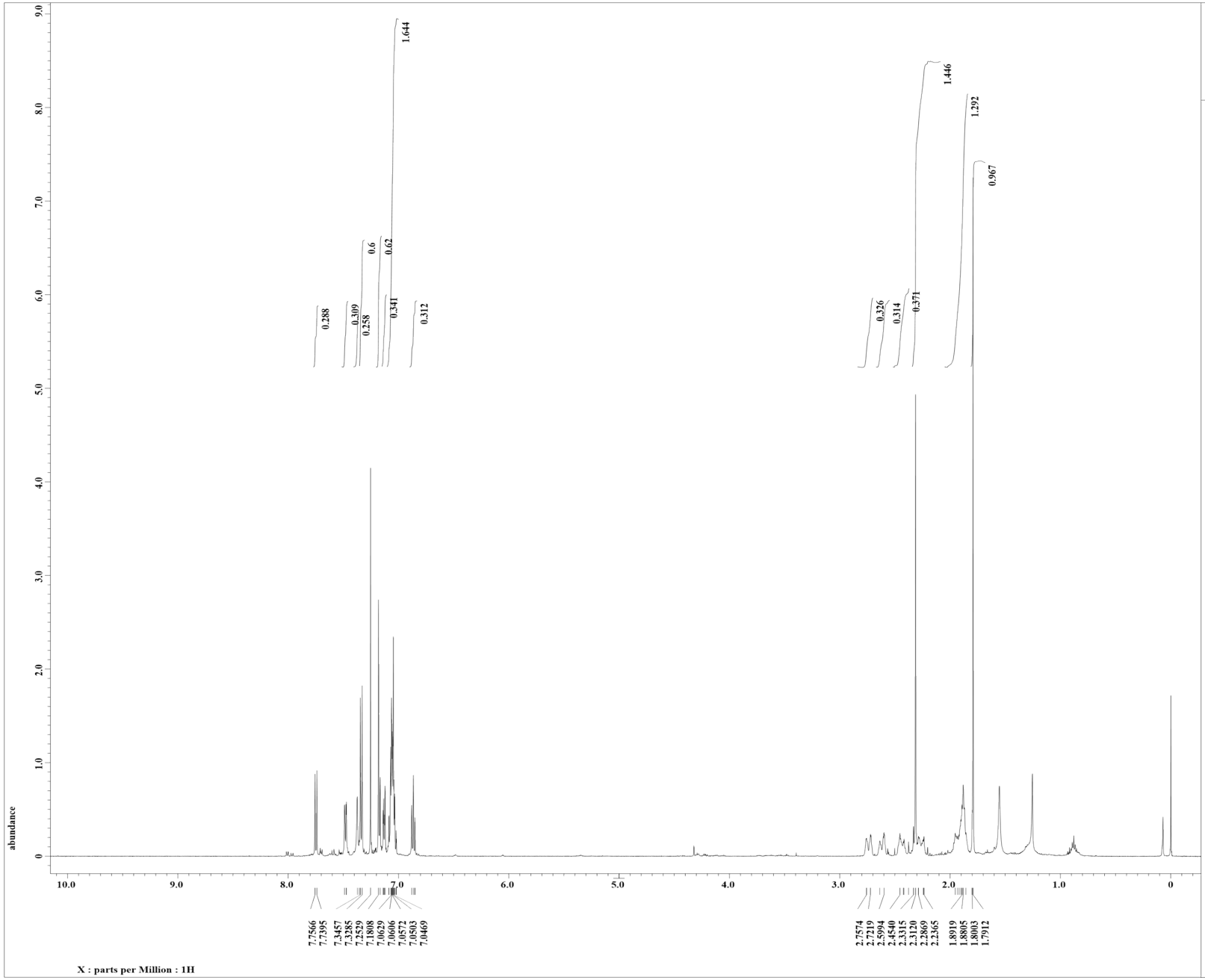
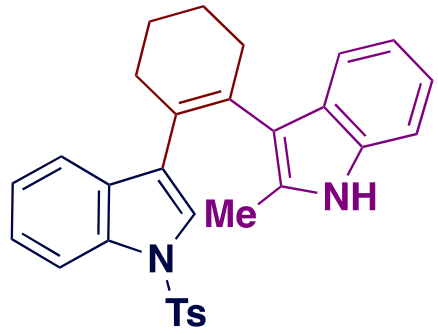
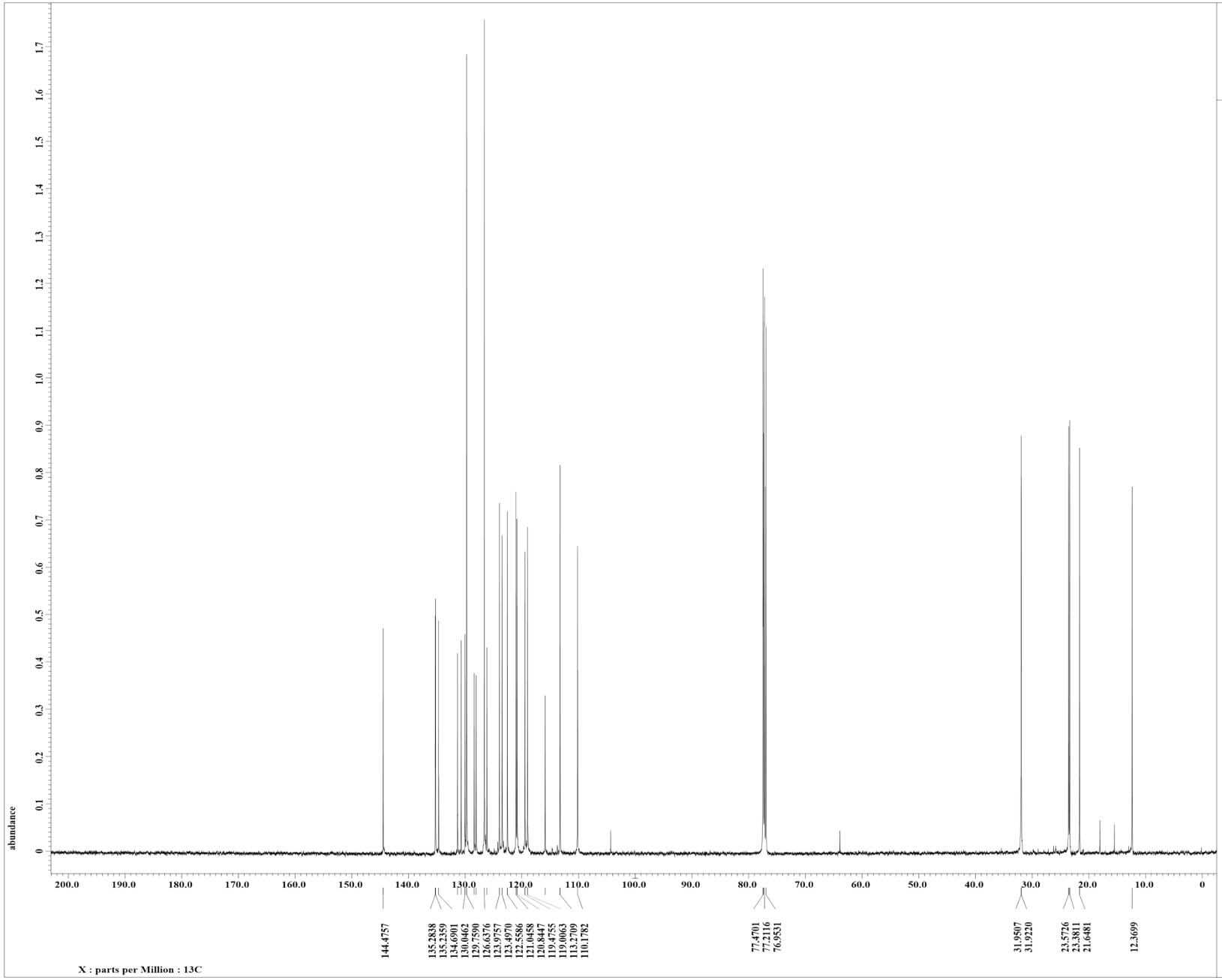
Ts



JEOL

```
Filename          = TA200530-modification
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#437062
Solvent           = CHLOROFORM-D
Creation_time     = 30-MAY-2020 11:30:25
Revision_time     = 30-MAY-2020 12:14:23
Current_time      = 30-MAY-2020 12:15:30

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 46
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 24.3[dC]
```



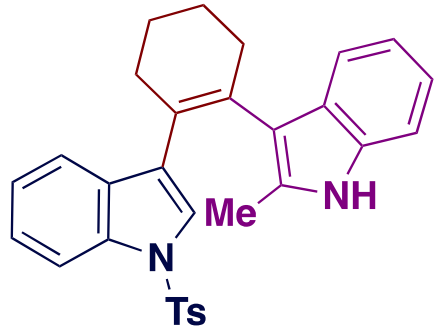


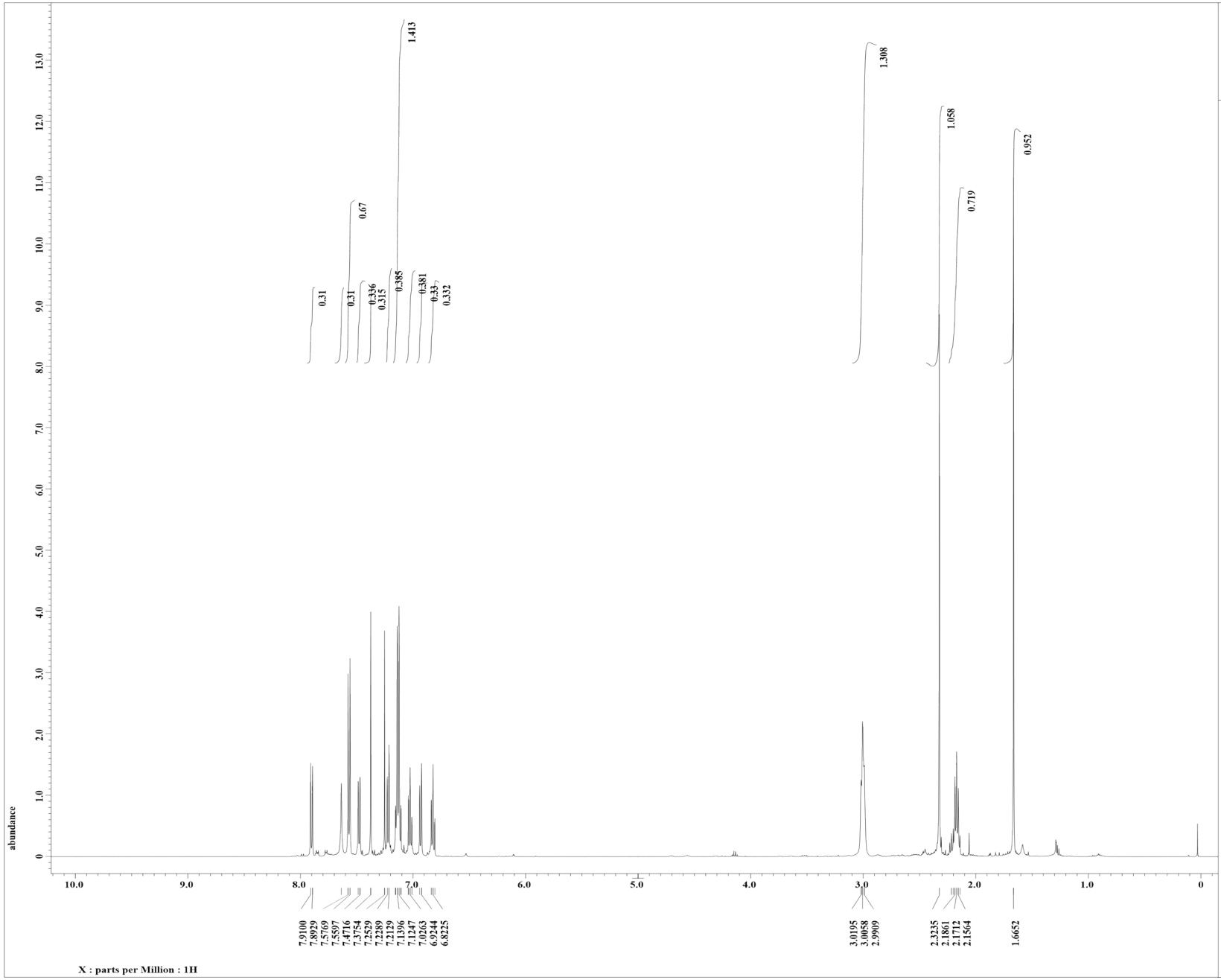
Filename = TA200530-modification
Author = delta
Experiment = single_pulse_dec
Sample_id = S#491370
Solvent = CHLOROFORM-D
Creation_time = 30-MAY-2020 15:22:43
Revision_time = 30-MAY-2020 16:04:49
Current_time = 30-MAY-2020 16:05:41

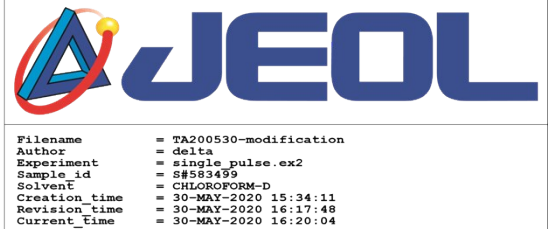
Content = cyclohexene
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 3020
Total_scans = 3020

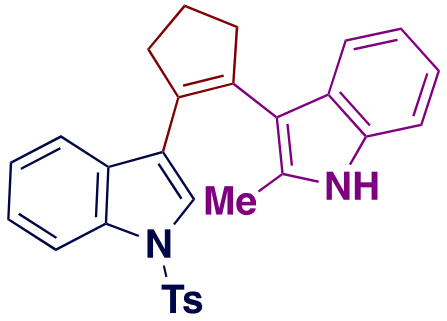
X_90_width = 10.1[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.36666667[us]
Irr_atn_dec = 21.51[dB]
Irr_atn_noe = 21.51[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get = 25.1[dC]

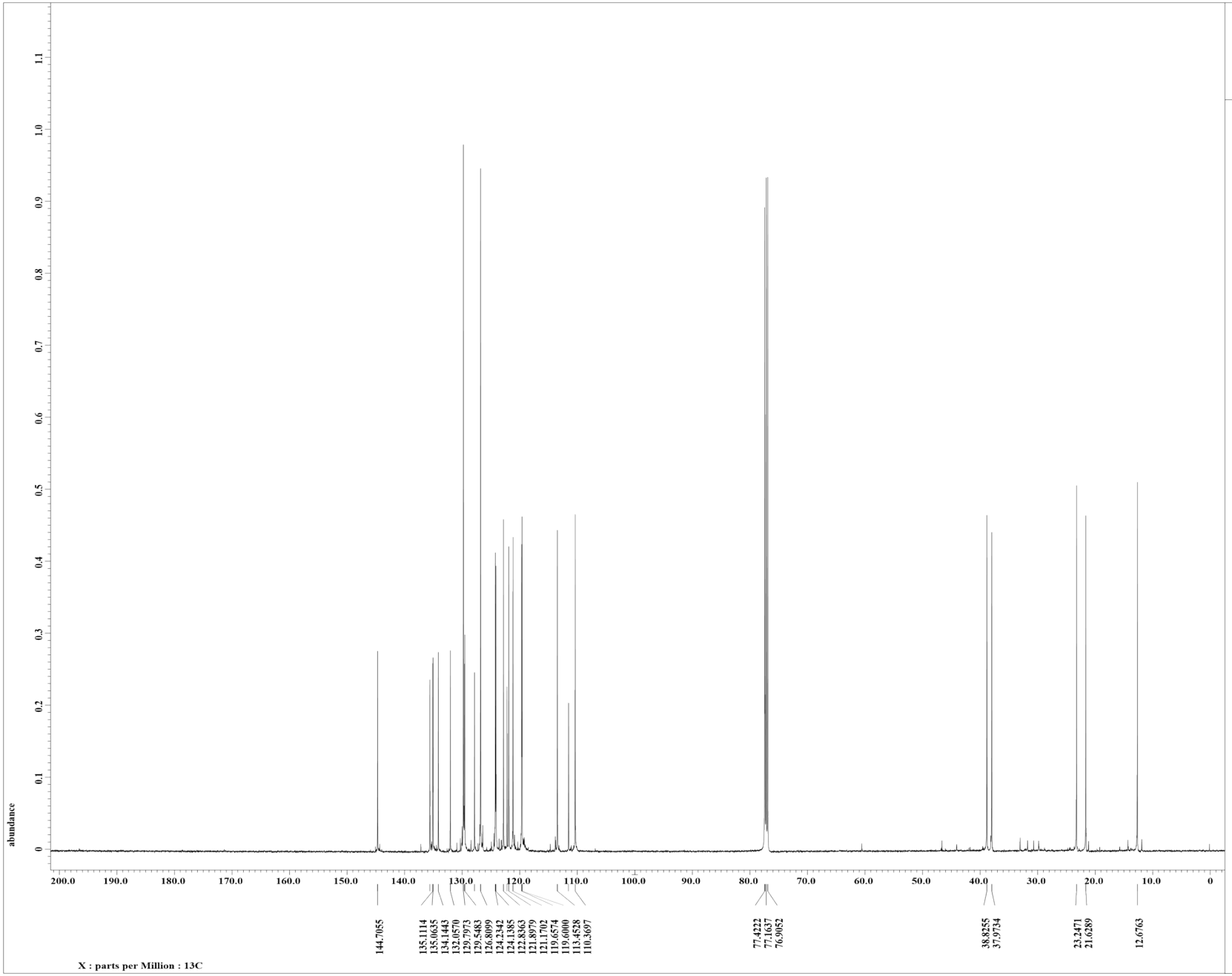






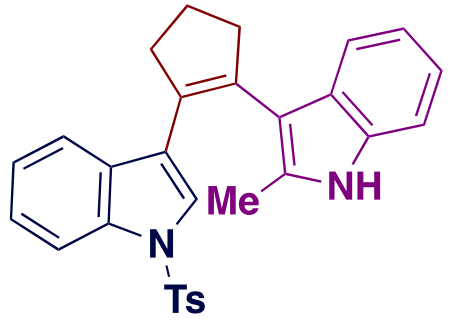
```
Filename          = TA200530-modification
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#583499
Solvent           = CHLOROFORM-D
Creation_time     = 30-MAY-2020 15:34:11
Revision_time     = 30-MAY-2020 16:17:48
Current_time      = 30-MAY-2020 16:20:04

Content           = cyclopentene
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 24.6[dC]
```

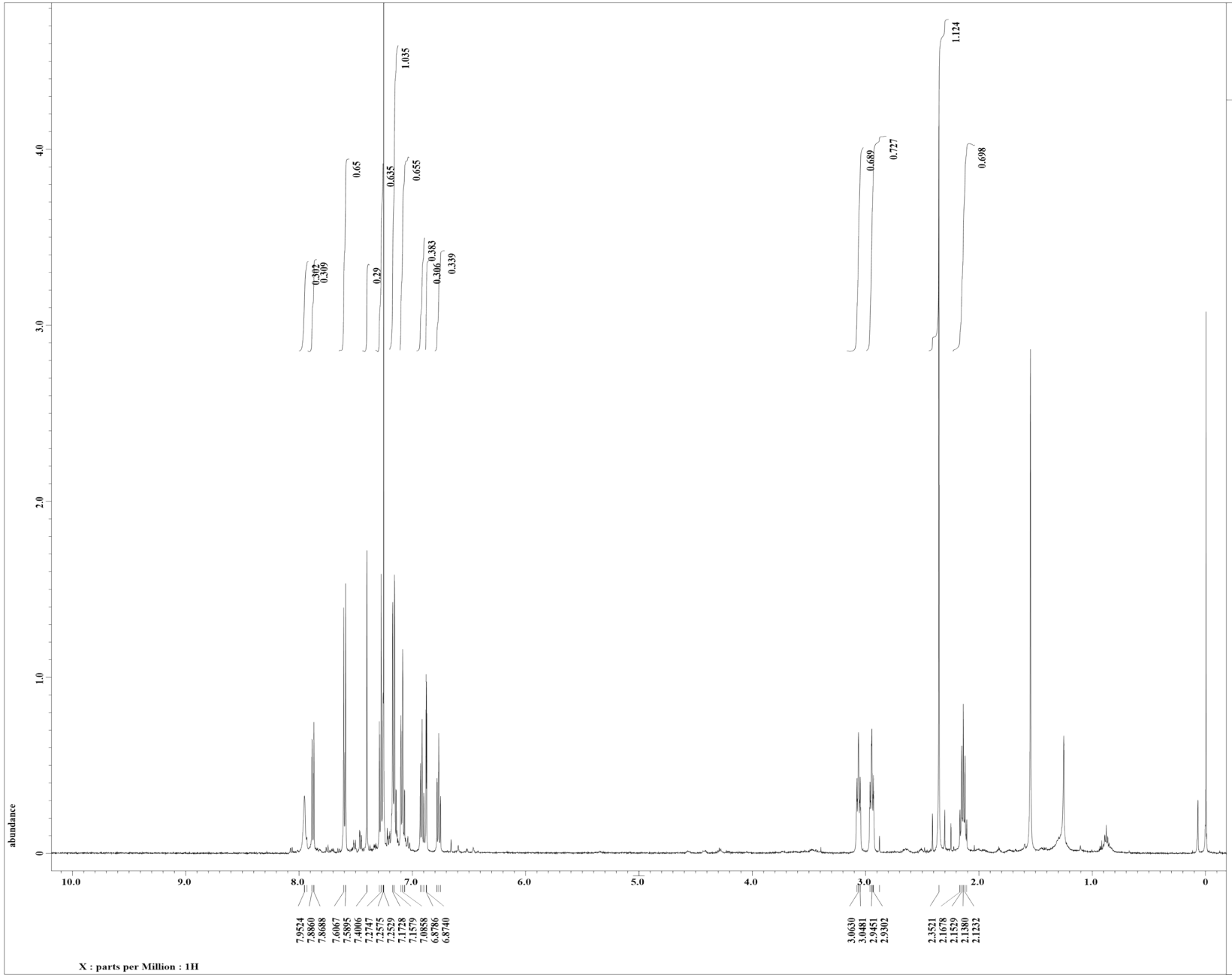


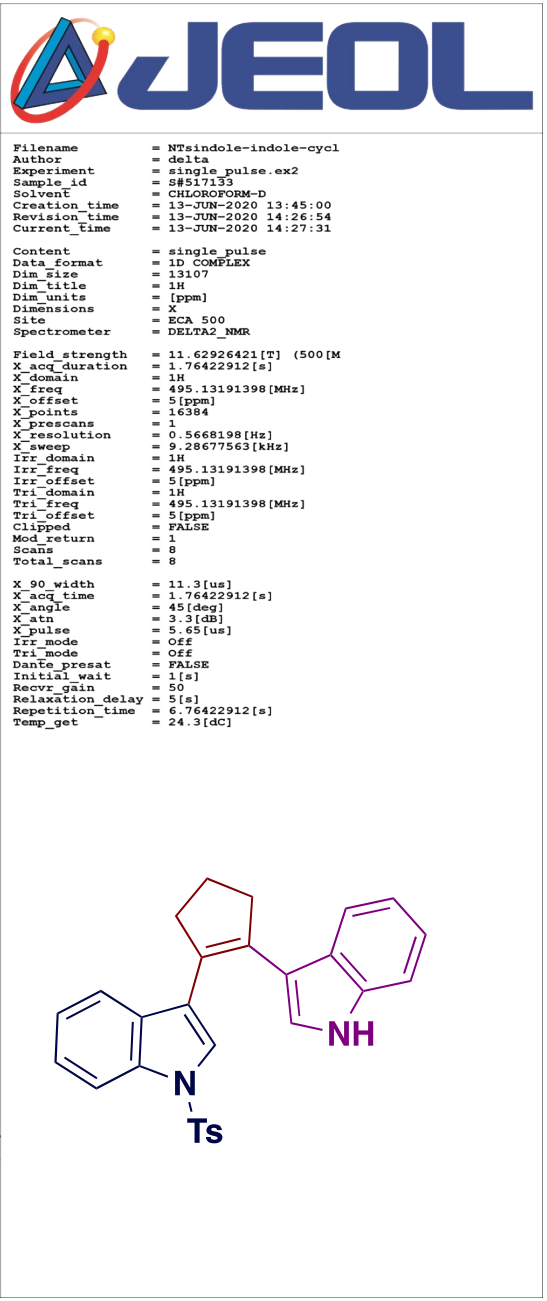


JEOL

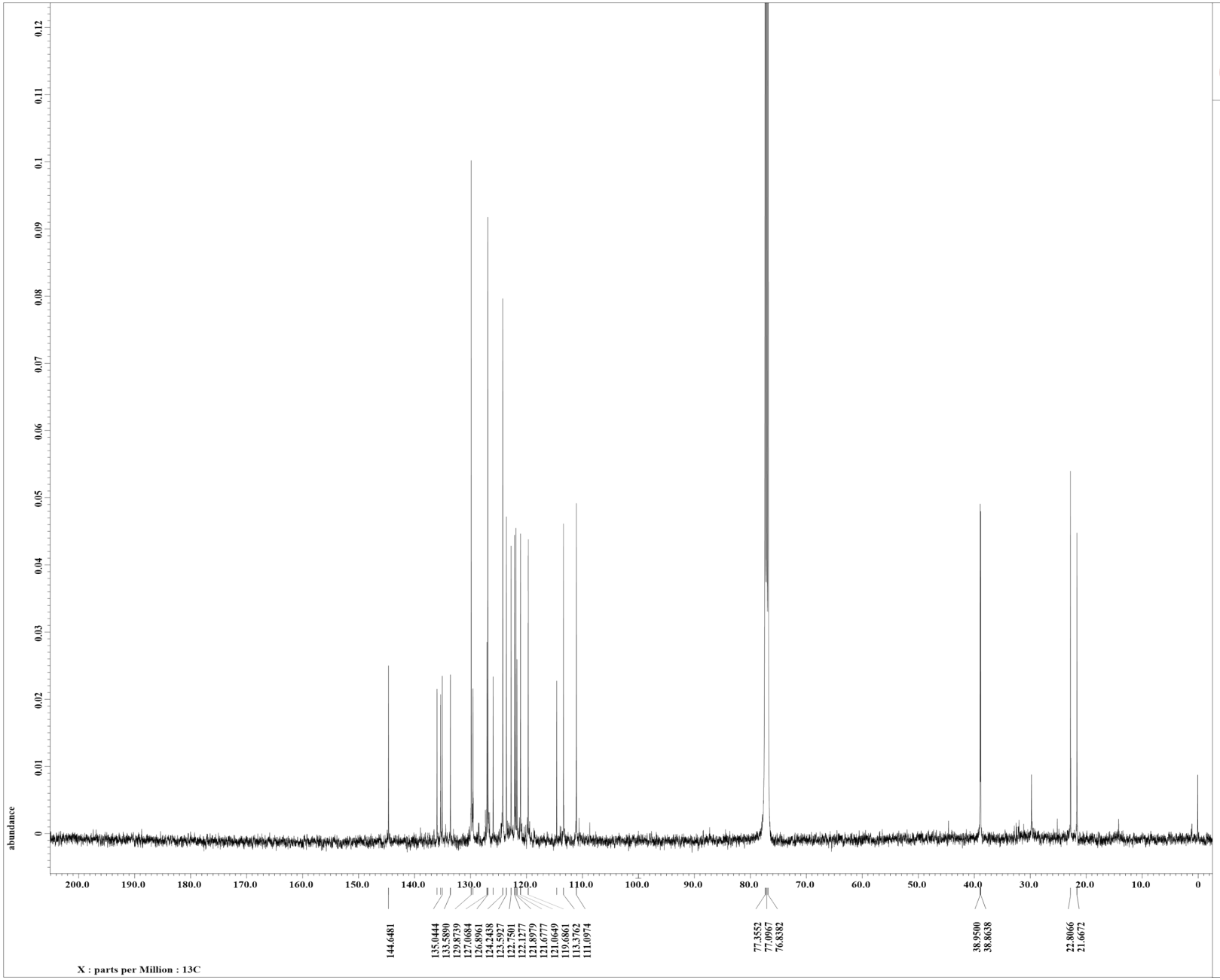
```
Filename          = TA200530-modification
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#585209
Solvent           = CHLOROFORM-D
Creation_time     =  1-JUN-2020 07:42:53
Revision_time     =  1-JUN-2020 08:24:27
Current_time      =  1-JUN-2020 08:26:11

Content           = cyclopentene
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 50864
Total_scans       = 50864

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 24.9[dC]
```



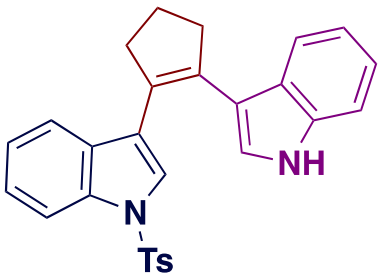


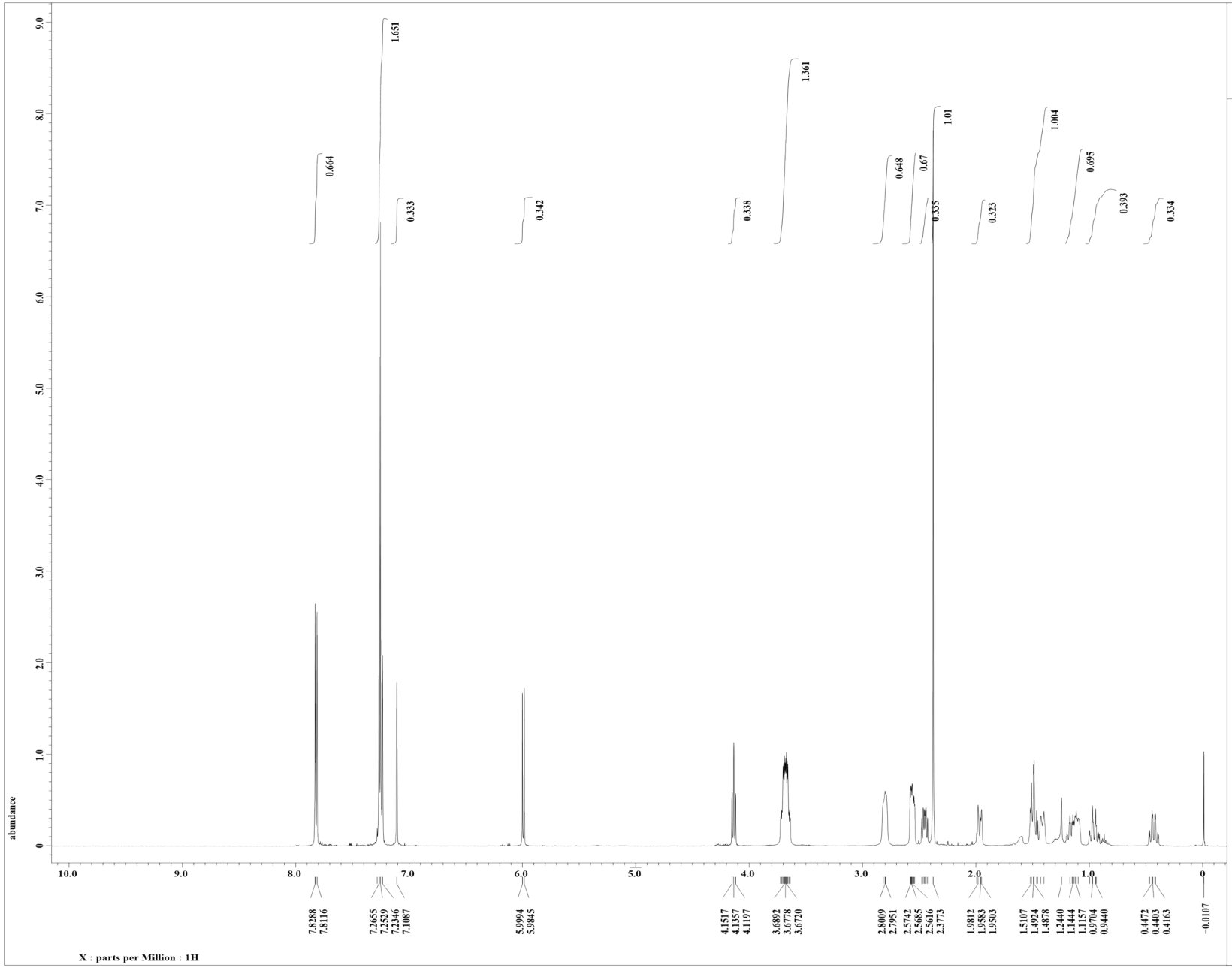


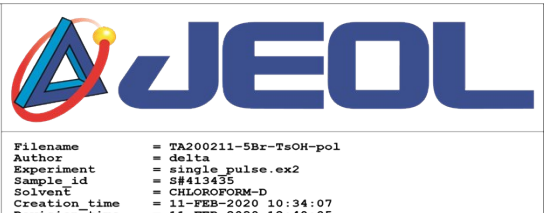
```
Filename          = NTsindole-indole-cycl
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#517133
Solvent           = CHLOROFORM-D
Creation_time     = 13-JUN-2020 13:45:00
Revision_time     = 13-JUN-2020 14:26:54
Current_time      = 13-JUN-2020 14:27:31

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 24.3[dC]
```



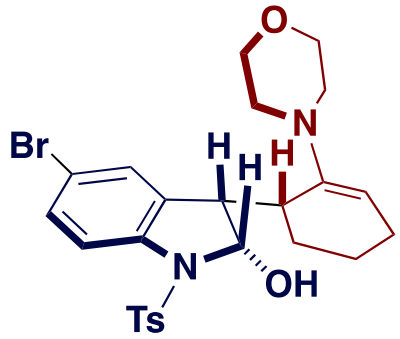

```
Filename          = NTsindole-indole-cycl
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#5185I3
Solvent           = CHLOROFORM-D
Creation_time     = 15-JUN-2020 07:18:27
Revision_time     = 15-JUN-2020 07:57:42
Current_time      = 15-JUN-2020 07:58:33

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 52657
Total_scans       = 52657

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 25.1[dC]
```

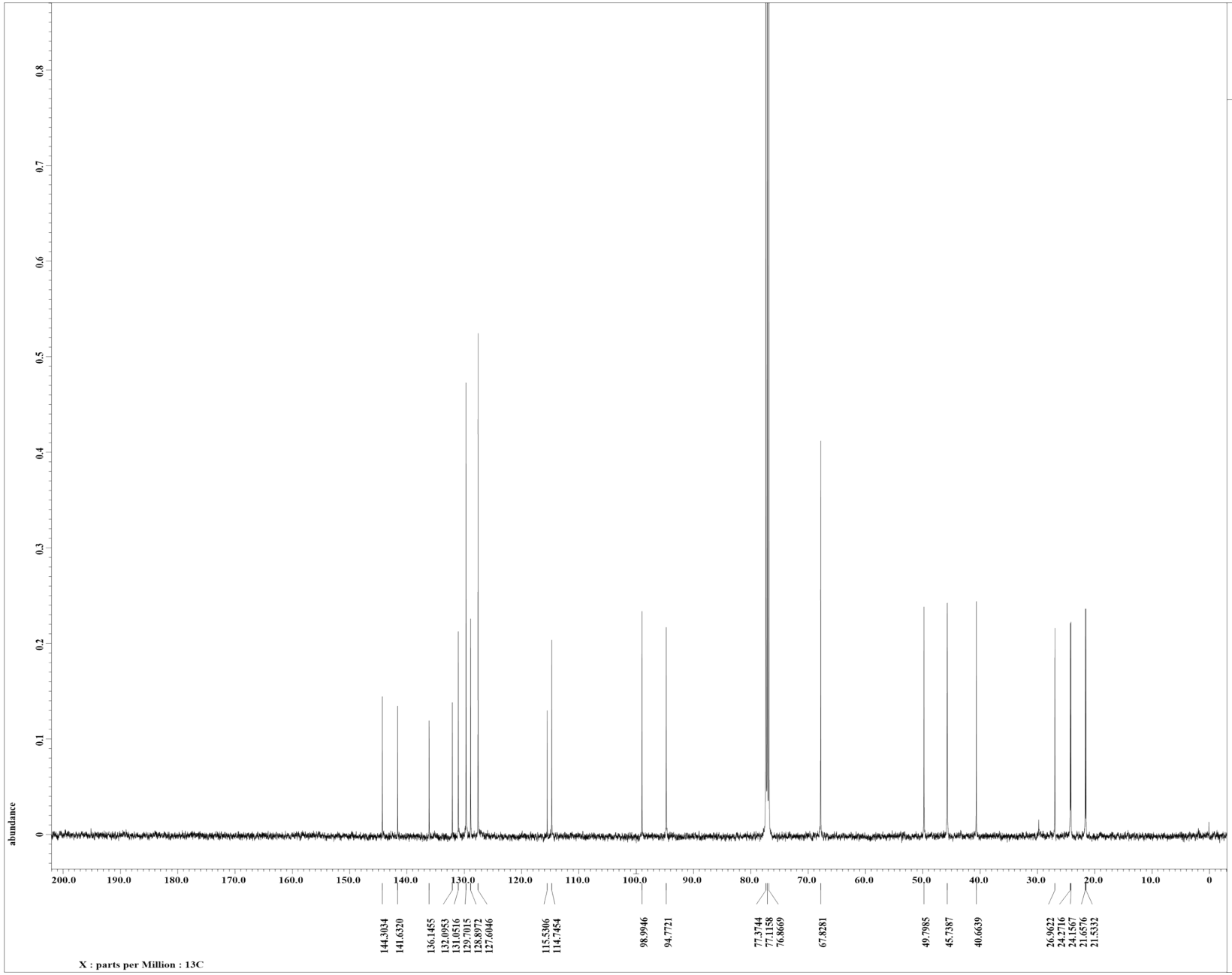




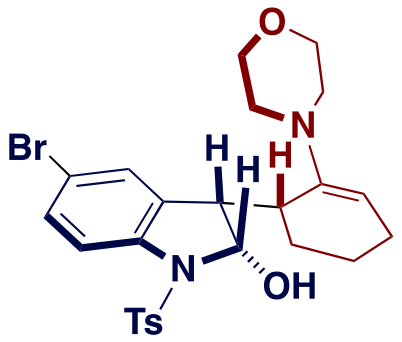


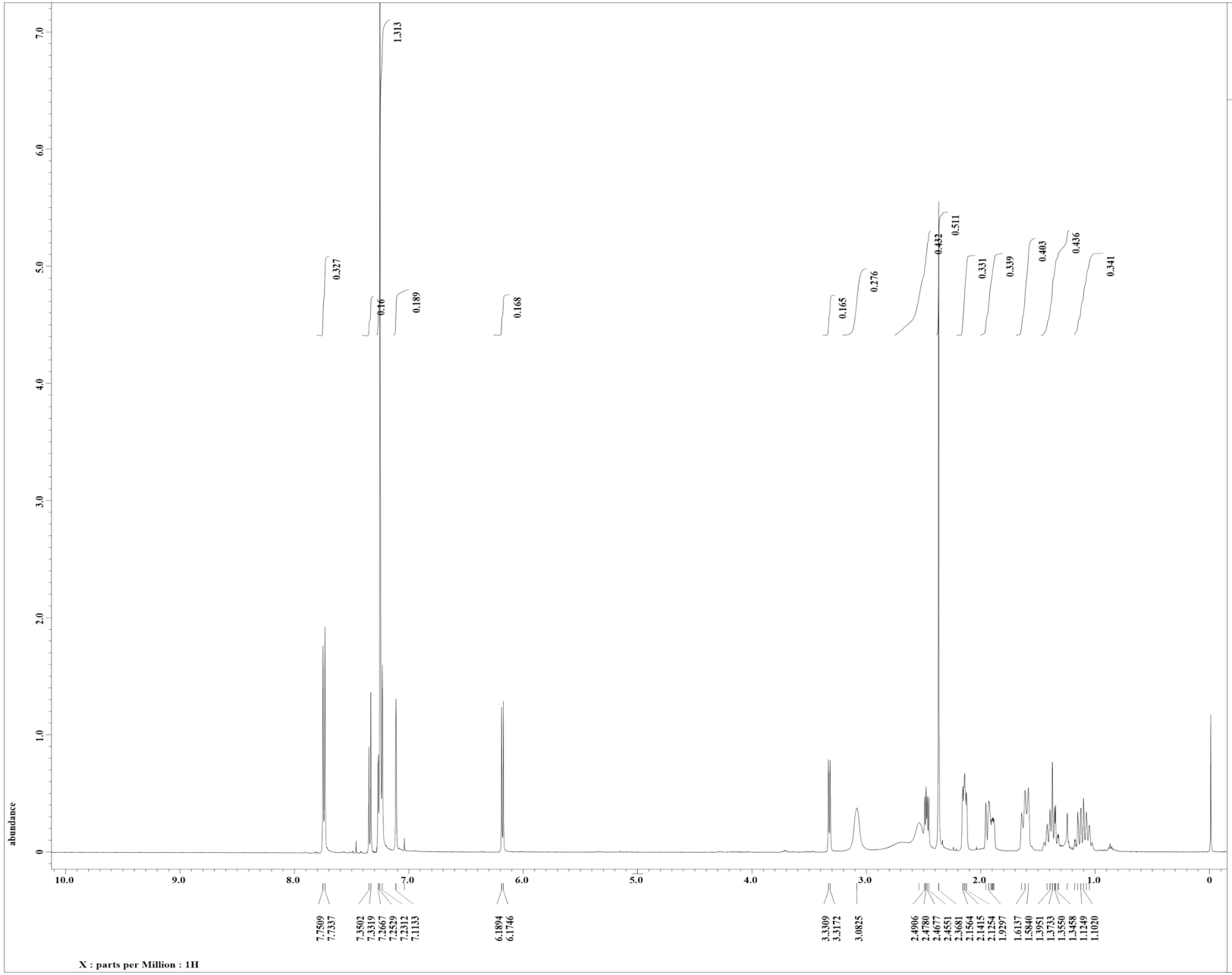
```
Filename          = TA200211-5Br-TsOH-pol
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#413435
Solvent           = CHLOROFORM-D
Creation_time     = 11-FEB-2020 10:34:07
Revision_time     = 11-FEB-2020 12:40:05
Current_time      = 11-FEB-2020 12:40:25

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.3[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.3[dB]
X_pulse           = 5.65[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 23[dC]
```






```
Filename          = TA200211-5Br-TsOH-pol
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#461522
Solvent           = CHLOROFORM-D
Creation_time     = 11-FEB-2020 14:10:54
Revision_time     = 11-FEB-2020 15:08:11
Current_time      = 11-FEB-2020 15:08:55

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 2901
Total_scans       = 2901

X_90_width        = 10.1[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.5[dB]
X_pulse           = 3.36666667[us]
Irr_atn_dec       = 21.51[dB]
Irr_atn_noe       = 21.51[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 23.7[dC]
```



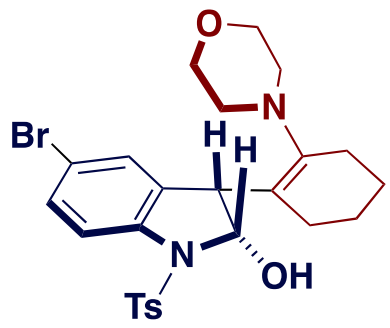


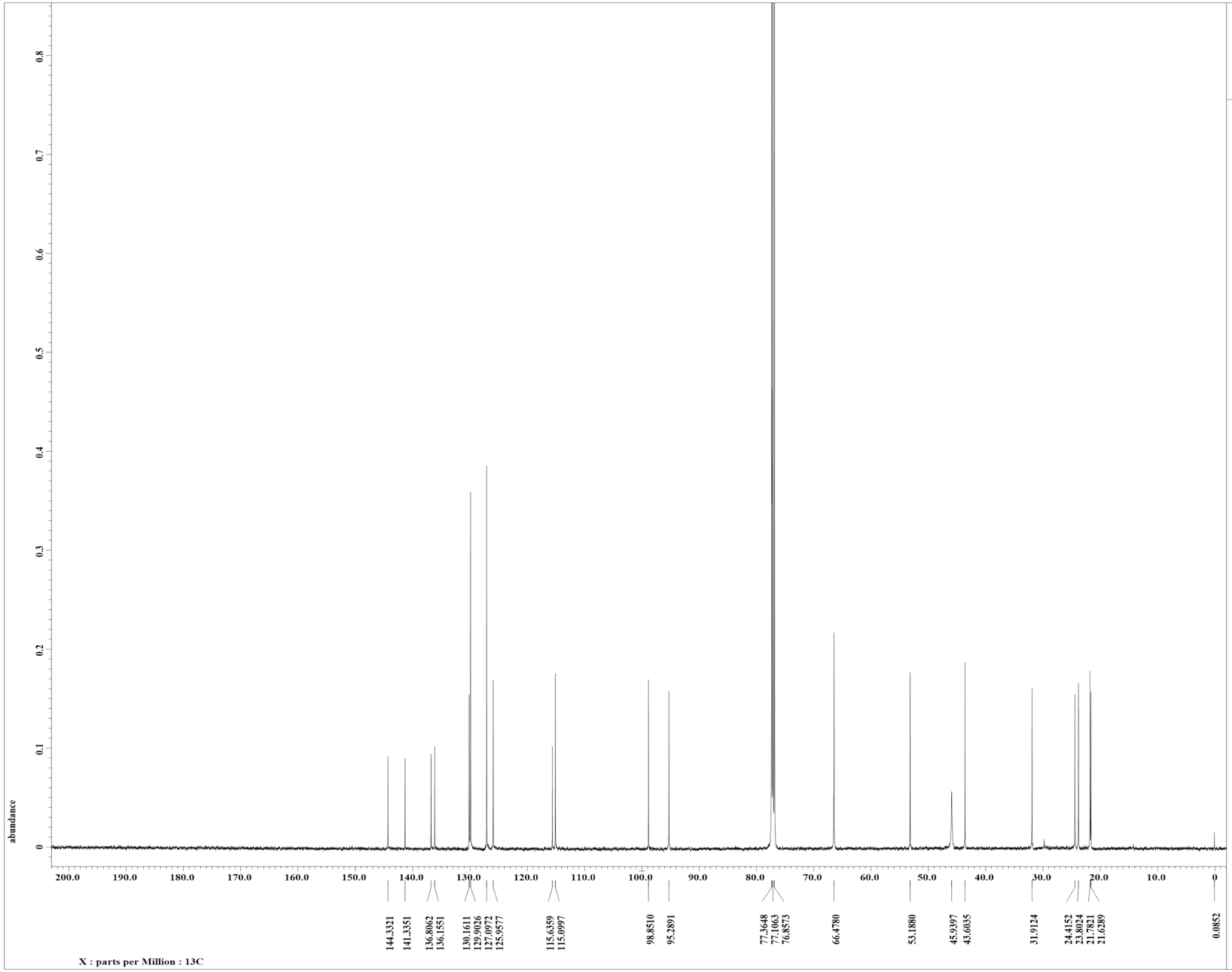
Filename = TA200210-5Br-TsOH-6.j
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#623049
Solvent = CHLOROFORM-D
Creation_time = 10-FEB-2020 16:23:33
Revision_time = 10-FEB-2020 17:27:55
Current_time = 10-FEB-2020 17:28:41

Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.3[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_pulse = 5.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 22.9[dC]





Filename = TA200210-5Br-TsOH-10.
Author = delta
Experiment = single_pulse_dec
Sample_id = S#753694
Solvent = CHLOROFORM-D
Creation_time = 11-FEB-2020 10:22:10
Revision_time = 11-FEB-2020 11:19:24
Current_time = 11-FEB-2020 11:20:55

Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 18212
Total_scans = 18212

X_90_width = 10.1[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.36666667[us]
Irr_atn_dec = 21.51[dB]
Irr_atn_noe = 21.51[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get = 23.5[dC]