Rapid Access to Indole–fused Bicyclo[2.2.2]octanones by Merging Umpolung Strategy and Molecular Iodine as A Green Catalyst

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SUPPORTING INFORMATION

Contents

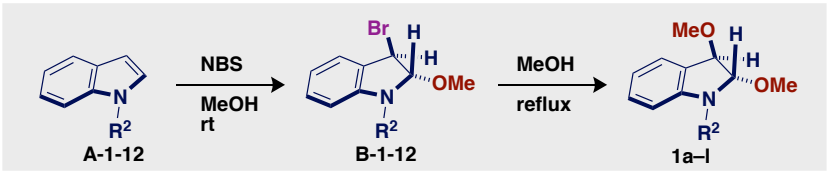
Experimental Section

1. General Experimental

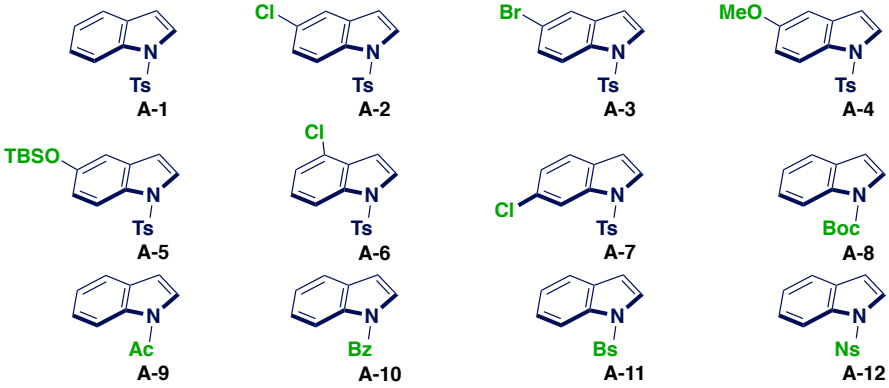
All reagents were weighed and handled in air at room temperature. Reactions were monitored by thin layer chromatography (TLC) carried out on a silica gel plates (60F-254) and visualized under UV illumination at 254 or 366 nm depending on the compounds. Extracts were dried over anhydrous $MgSO_4$. Solvents were removed by a rotary evaporator *in vacuo*. Column chromatography was performed on silica gel (Silica Gel 63–210 mesh, Kanto Chemical Co., Ltd.). The NMR experiments were performed with a JEOL JNM-ECA500 (500 MHz) spectrometer, and chemical shifts are expressed in ppm (δ) using residual solvent as an internal reference ($CDCl_3$, ^{1}H NMR: δ 7.25, ^{13}C NMR: δ 77.1). ^{1}H NMR data is represented as follows: Chemical shift (multiplicity, coupling constant(s) *J* in Herts (Hz), integration). The following abbreviations were used to explain NMR peak multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, ddd = doublet of doublet of doublets, br = broad. High resolution mass spectra (HRMS) were recorded on a JEOL JMS-T100LP mass spectrometers using electrospray ionization-time of flight (ESI-TOF) reflection experiments. All N-protected indoles are known products. The N-protected indoles **A1–12** were prepared by following a previous literature.[S1] 2-Methoxy-3-bromoindolines **B1–4**, **B6–10**, **B-12** were prepared by reported methods.[S2-3] 2,3-Dimethoxyindolines **1a-d**, **1f-j**, **1l** were prepared by reported methods.[S3]

2. Experimental Procedure

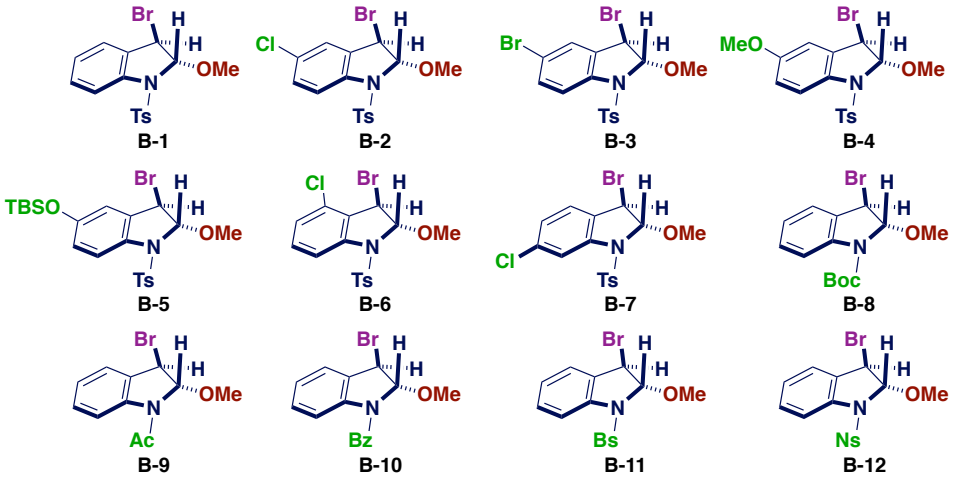
Synthesis of 2,3-Dimethoxyindolines 1



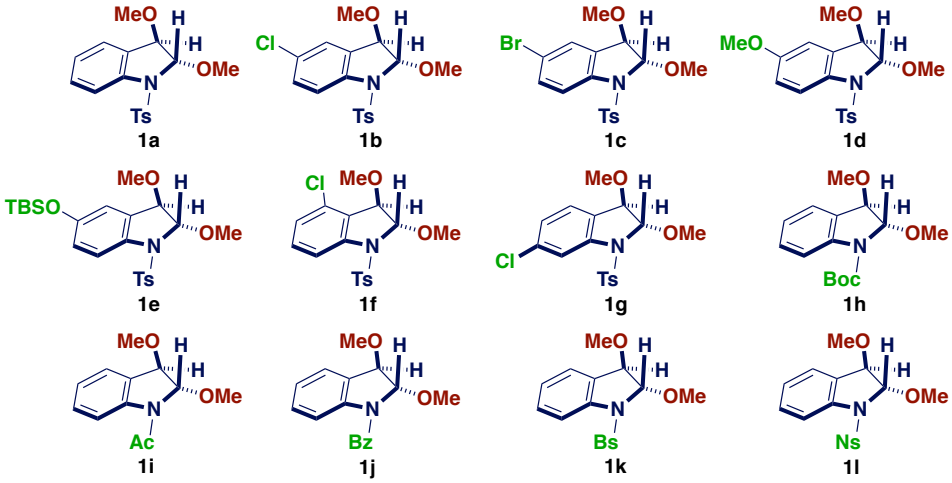
N-protected indoles



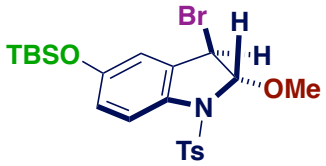
2-Methoxy-3-bromoindoline (MeOBINs)



2,3-Dimethoxyindolines (DiMeOINs)



trans-3-Bromo-2-methoxy-5-TBSO-1-tosylindoline (B-5)

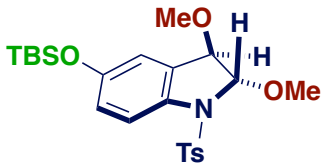


B-5

To a solution of N-Ts 5-TBSO-indole **A-5** (803 mg, 2 mmol) in MeOH (20 mL) was added NBS (392 mg, 2.2 mmol). The mixture was stirred at room temperature. After 1 h, Et_2O (10 mL) was dropwise added to the mixture and the mixture was stirred for 10 min. The resulting precipitate was separated by filtration, washed with MeOH, and dried *in vacuo* to give **B-5**.

782.1 mg, 76% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.62 (d, *J* = 8.6 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.80 (dd, *J* = 2.9, 9.2 Hz, 1H), 6.71 (d, *J* = 2.9 Hz, 1H), 5.51 (s, 1H), 4.83 (s, 1H), 3.57 (s, 3H), 2.28 (s, 3H), 0.94 (s, 9H), 0.15 (s, 3H), 0.14 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 153.6, 144.4, 135.2, 134.7, 132.9, 129.5, 127.8, 122.4, 118.3, 117.5, 100.3, 56.4, 47.3, 25.7, 21.6, 18.2, –4.4; HRMS (ESI) *m/z*: 534.0748, 536.0730 (Calcd for $C_{22}H_{30}BrNNaO_4SSi$ $[M+Na]^+$: 534.0746, 536.0725).

trans-2,3-Dimethoxy-5-TBSO-1-tosylindoline (1e)

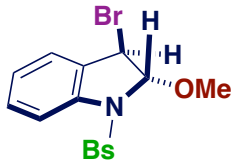


1e

A solution of **B-5** (513 mg, 1 mmol) in MeOH (15 mL) was stirred at 100 °C for 16 h. After addition of H_2O, the whole was extracted with AcOEt (3 x 25 mL), washed with brine (25 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/5–1/2) to give **1e**.

255.0 mg, 55% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.51 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 9.1 Hz, 1H), 7.11 (d, *J* = 8.1 Hz, 2H), 6.80 (dd, *J* = 9.2, 2.9 Hz, 1H), 6.72 (d, *J* = 2.3 Hz, 1H), 5.24 (s, 1H), 4.14 (s, 1H), 3.59 (s, 3H), 3.09 (s, 3H), 2.32 (s, 3H), 0.95 (s, 9H), 0.15 (s, 3H), 0.14 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 153.1, 143.9, 135.8, 135.0, 131.9, 129.9, 129.2, 128.0, 127.6, 122.0, 118.7, 118.3, 96.9, 84.1, 56.1, 25.7, 21.6, 18.2, –4.4; HRMS (ESI) *m/z*: 486.1745 (Calcd for $C_{23}H_{33}NNaO_5SSi$ $[M+Na]^+$: 486.1746).

trans-3-Bromo-2-methoxy-1-benzenesulfonyllindoline (B-11)

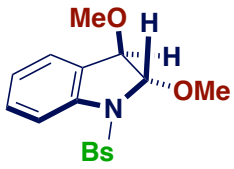


B-11

To a solution of N-Bs indole **A-11** (2.57 g, 10 mmol) in MeOH (200 mL) was added NBS (1.96 g, 11 mmol). The mixture was stirred at room temperature for 30 min. The resulting precipitate was separated by filtration, washed with MeOH, and dried *in vacuo* to give **B-11**.

2.99 g, 81% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.80 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.68 (d, *J* = 8.6 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.33 (t, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 7.5 Hz, 1H), 7.11 (td, *J* = 7.5, 1.2 Hz, 1H), 5.57 (s, 1H), 4.93 (s, 1H), 3.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 140.5, 138.2, 133.7, 131.5, 130.7, 129.0, 127.7, 126.3, 125.5, 117.1, 99.9, 56.4, 47.2, 28.8; HRMS (ESI) *m/z*: 389.9778, 391.9753 (Calcd for $C_{15}H_{14}BrNNaO_3S$ $[M+Na]^+$: 389.9775, 391.9755).

trans-2,3-Dimethoxy-1-benzenesulfonylindoline (1k)



1k

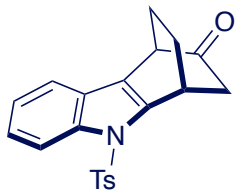
A solution of **B-11** (1.47 g, 4 mmol) in MeOH (100 mL) was stirred at 100 °C for 16 h. After addition of H_2O, the whole was extracted with AcOEt (3 x 50 mL), washed with brine (50 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (AcOEt/hexane = 1/5–1/2) to give **1k**.

753.7 mg, 59% yield. colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.69 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 8.6 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 3H), 7.28 (d, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 7.5 Hz, 1H), 5.31 (s, 1H), 4.24 (s, 1H), 3.59 (s, 3H), 3.12 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 140.8, 138.0, 133.3, 130.6, 130.5, 128.7, 127.5, 126.9, 124.9, 117.5, 96.6, 83.8, 56.1, 56.0; HRMS (ESI) *m/z*: 342.0776 (Calcd for $C_{16}H_{17}NNaO_4S$ $[M+Na]^+$: 342.0776).

General Procedure for the Iodine-catalyzed Cascade Reaction of DiMeOINs (1) with 2 (Scheme 2 and 3)

To a solution of **1** (0.5 mmol) and **2** (0.75 mmol) in MeCN (10 mL) was added I_2 (12.7 mg, 0.05 mmol). The mixture was stirred at 100 °C. After indicated time (Scheme 2), the mixture was cooled to room temperature and then concentrated *in vacuo*. The crude residue was directly purified by silica gel column chromatography ($CHCl_3$/hexane = 1/2–2/1) to give **3**.

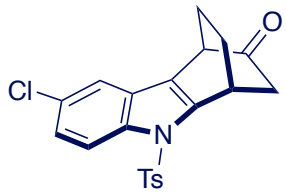
Rel-(1*R*,4*R*)-9-tosyl-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3aa)



3aa

135.8 mg, 74% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.18 (d, *J* = 8.6 Hz, 1H), 7.68 (d, *J* = 8.9 Hz, 2H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.30 (td, *J* = 7.5, 1.2 Hz, 1H), 7.26 (td, *J* = 7.5, 1.2 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 4.41 (t, *J* = 2.9 Hz, 1H), 3.89 (t, *J* = 2.9 Hz, 1H), 2.33 (s, 3H), 2.30 (dd, *J* = 18.3, 2.9 Hz, 1H), 2.05-2.11 (m, 2H), 1.98-2.03 (m, 1H), 1.58-1.69 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.4, 145.3, 141.7, 136.6, 135.8, 130.1, 127.1, 126.4, 124.3, 123.9, 118.3, 118.2, 114.9, 45.9, 41.6, 32.1, 26.3, 23.8, 21.7; HRMS (ESI) *m/z*: 388.0980 (Calcd for $C_{21}H_{19}NNaO_3S$ $[M+Na]^+$: 388.0983).

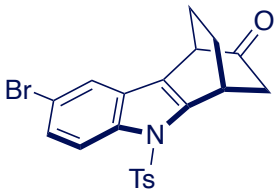
***Rel*-(1*R*,4*R*)-6-chloro-9-tosyl-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3ba)**



3ba

112.2 mg, 56% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.09 (d, *J* = 9.2 Hz, 1H), 7.66 (d, *J* = 8.6 Hz, 2H), 7.38 (d, *J* = 1.7 Hz, 1H), 7.25 (dd, *J* = 9.2, 2.3 Hz, 1H), 7.21 (d, *J* = 8.6 Hz, 2H), 4.38 (t, *J* = 2.9 Hz, 1H), 3.84 (t, *J* = 2.9 Hz, 1H), 2.34 (s, 3H), 2.30 (dd, *J* = 18.9, 2.9 Hz, 1H), 1.98-2.12 (m, 3H), 1.56-1.67 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 208.8, 145.6, 143.2, 135.5, 134.9, 130.3, 129.8, 128.3, 126.4, 124.4, 118.0, 117.6, 115.8, 45.8, 41.3, 32.2, 26.1, 23.7, 21.7; HRMS (ESI) *m/z*: 422.0597, 424.0563 (Calcd for $C_{21}H_{18}ClNNaO_3S$ $[M+Na]^+$: 422.0594, 424.0564).

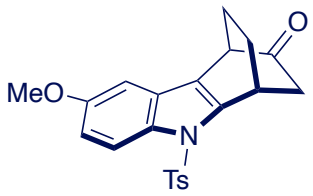
***Rel*-(1*R*,4*R*)-6-bromo-9-tosyl-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3ca)**



3ca

89.4 g, 40% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.05 (d, *J* = 9.2 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 1.7 Hz, 1H), 7.39 (dd, *J* = 9.2, 2.3 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 4.39 (t, *J* = 2.9 Hz, 1H), 3.84 (t, *J* = 2.9 Hz, 1H), 2.35 (s, 3H), 2.30 (dd, *J* = 18.4, 2.3 Hz, 1H), 1.99-2.12 (m, 3H), 1.57-1.67 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 208.7, 145.7, 143.0, 135.5, 135.3, 130.3, 128.8, 127.1, 126.4, 121.0, 117.5, 117.5, 116.2, 45.8, 41.3, 32.2, 26.1, 23.7, 21.7; HRMS (ESI) *m/z*: 466.0090, 468.0068 (Calcd for $C_{21}H_{18}BrNNaO_3S$ $[M+Na]^+$: 466.0088, 468.0068).

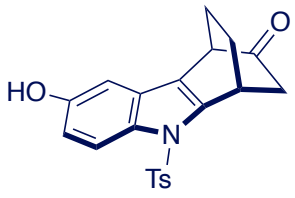
***Rel*-(1*R*,4*R*)-6-methoxy-9-tosyl-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3da)[S4]**



3da

140.4 mg, 69% yield. colorless oil ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.06 (d, *J* = 8.6 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.1 Hz, 2H), 6.90 (dd, *J* = 9.2, 2.9 Hz, 1H), 6.85 (d, *J* = 2.9 Hz, 1H), 4.37 (t, *J* = 2.9 Hz, 1H), 3.85 (t, *J* = 3.3 Hz, 1H), 3.82 (s, 3H), 2.33 (s, 3H), 2.29 (dd, *J* = 18.3, 2.9 Hz, 1H), 1.97-2.12 (m, 3H), 1.57-1.68 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.3, 156.9, 145.2, 142.5, 135.7, 131.2, 130.1, 128.2, 126.4, 118.4, 115.8, 113.0, 100.9, 55.7, 45.9, 41.6, 32.2, 26.2, 23.8, 21.7; HRMS (ESI) *m/z*: 418.1089 (Calcd for $C_{22}H_{21}NNaO_4S$ $[M+Na]^+$: 354.0106, 418.1089).

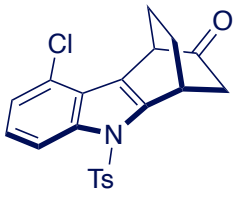
***Rel*-(1*R*,4*R*)-6-hydroxy-9-tosyl-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3ea')**



3ea'

129.3 mg, 68% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.00 (d, *J* = 7.7 Hz, 1H), 7.63 (d, *J* = 8.6 Hz, 2H), 7.18 (d, *J* = 8.6 Hz, 2H), 6.77-6.84 (m, 2H), 5.97 (br s, 1H), 4.35 (s, 1H), 3.80 (s, 1H), 2.32 (s, 3H), 2.15-2.27 (m, 1H), 1.95-2.12 (m, 3H), 1.55-1.64 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 210.6, 153.1, 145.3, 142.7, 135.6, 131.2, 130.1, 128.4, 126.4, 118.0, 115.8, 113.2, 103.5, 45.9, 41.7, 32.1, 26.1, 23.7, 21.7; HRMS (ESI) *m/z*: 404.0930 (Calcd for $C_{21}H_{19}NNaO_4S$ $[M+Na]^+$: 404.0932).

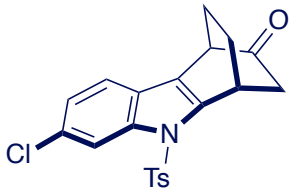
***Rel*-(1*R*,4*R*)-5-chloro-9-tosyl-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3fa)**



3fa

104.4 mg, 52% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.10-8.14 (m, 1H), 7.68 (d, *J* = 8.6 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 5.2 Hz, 2H), 4.46 (t, *J* = 2.9 Hz, 1H), 4.43 (t, *J* = 4.9 Hz, 1H), 2.36 (s, 3H), 2.30 (dd, *J* = 18.3, 2.3 Hz, 1H), 1.97-2.13 (m, 3H), 1.56-1.76 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.3, 145.7, 142.8, 137.4, 135.6, 130.3, 126.5, 125.6, 125.0, 124.6, 124.5, 117.5, 113.3, 46.7, 41.1, 32.0, 25.8, 23.9, 21.7; HRMS (ESI) *m/z*: 422.0592, 424.0564 (Calcd for $C_{21}H_{18}ClNNaO_3S$ $[M+Na]^+$: 422.0594, 424.0564).

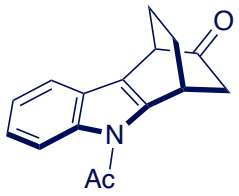
***Rel*-(1*R*,4*R*)-7-chloro-9-tosyl-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3ga)**



3ga

89.6 mg, 45% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.21 (d, *J* = 1.7 Hz, 1H), 7.68 (d, *J* = 8.6 Hz, 2H), 7.32 (d, *J* = 8.6 Hz, 1H), 7.24 (d, *J* = 8.6 Hz, 2H), 7.23 (dd, *J* = 8.0, 1.7 Hz, 1H), 4.38 (t, *J* = 2.9 Hz, 1H), 3.86 (t, *J* = 4.9 Hz, 1H), 2.36 (s, 3H), 2.30 (dd, *J* = 17.8, 2.3 Hz, 1H), 1.98-2.12 (m, 3H), 1.56-1.68 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.0, 145.7, 142.2, 136.8, 135.6, 130.3, 130.1, 126.5, 125.6, 124.5, 118.8, 117.9, 115.1, 45.8, 41.4, 32.1, 26.2, 23.7, 21.7; HRMS (ESI) *m/z*: 422.0595, 424.0561 (Calcd for $C_{21}H_{18}ClNNaO_3S$ $[M+Na]^+$: 422.0594, 424.0564).

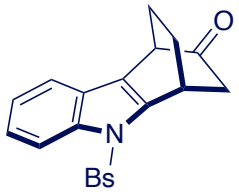
***Rel*-(1*R*,4*R*)-9-acetyl-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3ia)**



3ia

77.6 mg, 69% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.04 (d, *J* = 7.5 Hz, 1H), 7.48 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.27-7.32 (m, 2H), 4.41 (t, *J* = 2.9 Hz, 1H), 3.97 (t, *J* = 3.6 Hz, 1H), 2.77 (s, 3H), 2.33 (d, *J* = 2.3 Hz, 2H), 2.13-2.20 (m, 1H), 1.95-2.06 (m, 1H), 1.71-1.79 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.6, 169.6, 142.3, 136.3, 127.2, 124.4, 123.7, 118.3, 118.1, 115.9, 45.7, 41.6, 33.6, 27.1, 26.2, 23.6; HRMS (ESI) *m/z*: 276.1005 (Calcd for $C_{16}H_{15}NNaO_2$ $[M+Na]^+$: 276.1000).

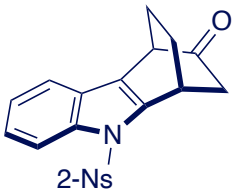
***Rel*-(1*R*,4*R*)-9-(phenylsulfonyl)-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3ka)**



3ka

133.4 mg, 69% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.19 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 7.5 Hz, 2H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.32 (td, *J* = 7.5, 1.2 Hz, 1H), 7.27 (d, *J* = 8.1 Hz, 1H), 4.41 (t, *J* = 2.9 Hz, 1H), 3.90 (t, *J* = 2.9 Hz, 1H), 2.31 (dd, *J* = 18.4, 2.3 Hz, 1H), 1.98-2.13 (m, 3H), 1.57-1.69 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.3, 141.6, 138.8, 136.7, 134.2, 129.6, 127.1, 126.4, 124.4, 124.0, 118.5, 118.2, 114.9, 45.9, 41.6, 32.1, 26.3, 23.8; HRMS (ESI) *m/z*: 374.0826 (Calcd for $C_{20}H_{17}NNaO_3S$ $[M+Na]^+$: 374.0827).

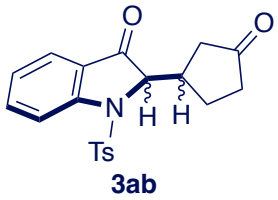
***Rel*-(1*R*,4*R*)-9-((2-nitrophenyl)sulfonyl)-2,3,4,9-tetrahydro-1*H*-1,4-ethanocarbazol-10-one (3la)**



3la

43.6 mg, 22% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.90 (d, *J* = 7.5 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.61 (t, *J* = 8.0 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.27-7.32 (m, 2H), 4.24 (t, *J* = 2.9 Hz, 1H), 3.98 (t, *J* = 2.9 Hz, 1H), 2.21-2.33 (m, 2H), 2.10-2.17 (m, 1H), 1.97-2.04 (m, 1H), 1.64-1.75 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.4, 147.8, 142.8, 136.7, 134.9, 133.1, 132.7, 129.2, 126.8, 125.4, 124.6, 124.4, 118.6, 118.4, 114.6, 46.0, 41.6, 32.4, 26.2, 23.9; HRMS (ESI) *m/z*: 419.0689 (Calcd for $C_{20}H_{16}N_2NaO_5S$ $[M+Na]^+$: 419.0687).

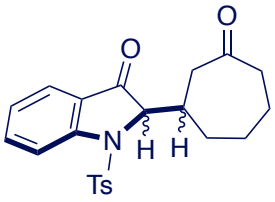
2-(3-Oxocyclopentyl)-1-tosylindolin-3-one (3ab)



3ab

149.1 mg, 81% yield (dr = 2:1). colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.05 (d, *J* = 8.6 Hz, 2/3H), 8.04 (d, *J* = 8.6 Hz, 1/3H), 7.70 (td, *J* = 7.5, 1.2 Hz, 1H), 7.56 (d, *J* = 6.9 Hz, 1H), 7.50 (d, *J* = 8.6 Hz, 4/3 H), 7.48 (d, *J* = 8.6 Hz, 2/3 H), 4.13 (d, *J* = 4.0 Hz, 2/3H), 4.09 (d, *J* = 4.6 Hz, 1/3H), 3.02-3.11 (m, 2/3H), 2.93-3.01 (m, 1/3H), 2.40-2.48 (m, 1H), 2.33 (s, 3H), 2.29-2.37 (m, 4/3H), 2.20-2.27 (m, 4/3H), 1.99-2.18 (m, 5/3H), 1.83-1.93 (m, 2/3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 216.8, 216.7, 198.4, 198.3, 153.8, 153.7, 145.4, 137.5, 137.4, 132.8, 132.7, 130.1, 127.4, 126.2, 126.0, 125.7, 125.6, 124.4, 118.7, 118.4, 68.5, 68.1, 40.7, 40.4, 40.3, 39.4, 39.3, 38.3, 38.2, 38.1, 25.1, 24.1, 21.6; HRMS (ESI) *m/z*: 492.0930 (Calcd for $C_{20}H_{19}NNaO_4S$ $[M+Na]^+$: 492.0932).

2-(3-Oxocycloheptyl)-1-tosylindolin-3-one (3ac)

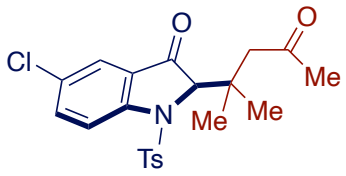


3ac

153.4 mg, 77% yield (dr = 2:1). colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.08 (d, *J* = 8.6 Hz, 2/3H), 8.01 (d, *J* = 8.6 Hz, 1/3H), 7.65-7.70 (m, 1H), 7.54-7.57 (m, 3H), 7.18-7.22 (m, 3H), 3.90 (d, *J* = 3.4 Hz, 1/3H), 3.80 (d, *J* = 4.0 Hz, 2/3H), 2.74-2.82 (m, 1H), 2.42-2.58 (m, 4H), 2.29-2.40 (m, 1H), 2.34 (s, 3H), (1.08-1.93 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 212.7, 212.6, 197.8, 197.7, 153.7, 148.5, 145.3, 139.9, 137.4, 137.3, 133.1, 133.0, 130.1, 127.4, 127.3, 125.9, 125.2, 125.1, 124.2, 117.7, 117.5, 70.9, 70.7, 50.0, 45.9, 44.2, 43.9, 43.8, 43.7, 40.1, 39.6, 38.2, 37.5, 32.4, 30.3, 29.5, 29.2, 29.0, 27.3, 24.9, 24.4, 24.1, 24.0, 21.6, 21.5; HRMS (ESI) *m/z*: 420.1243 (Calcd for

$C_{22}H_{23}NNaO_4S$ [M+Na]$^+$: 420.1245).

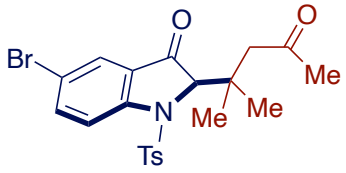
5-Chloro-2-(2-methyl-4-oxopentan-2-yl)-1-tosylindolin-3-one (3cf)



3bf

139.0 mg, 66% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.99 (d, *J* = 8.6 Hz, 1H), 7.61 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.41 (d, *J* = 2.3 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.64 (s, 1H), 4.71 (s, 1H), 2.92 (d, *J* = 18.3 Hz, 1H), 2.57 (d, *J* = 18.4 Hz, 1H), 2.32 (s, 3H), 2.19 (s, 3H), 1.00 (s, 3H), 0.97 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 207.7, 198.8, 152.9, 145.2, 136.3, 132.1, 131.8, 130.0, 129.9, 127.8, 123.2, 121.8, 71.6, 51.4, 38.2, 31.2, 25.4, 22.9, 21.6; HRMS (ESI) *m/z*: 442.0850, 444.0826 (Calcd for $C_{21}H_{22}ClNNaO_4S$ [M+Na]$^+$: 442.0856, 444.0826).

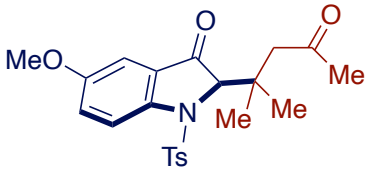
5-Bromo-2-(2-methyl-4-oxopentan-2-yl)-1-tosylindolin-3-one (3bf)



3cf

150.2 mg, 65% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.92 (d, *J* = 8.6 Hz, 1H), 7.74 (dd, *J* = 9.2, 2.3 Hz, 1H), 7.57 (d, *J* = 2.3 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.6 Hz, 2H), 4.64 (s, 1H), 4.70 (s, 1H), 2.91 (d, *J* = 18.3 Hz, 1H), 2.56 (d, *J* = 18.3 Hz, 1H), 2.32 (s, 3H), 2.19 (s, 3H), 1.00 (s, 3H), 0.97 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 207.6, 198.6, 153.3, 145.2, 139.1, 131.8, 130.2, 130.0, 127.8, 126.3, 122.1, 119.6, 71.5, 51.4, 38.2, 31.2, 25.4, 22.9, 21.6; HRMS (ESI) *m/z*: 486.0348, 488.0325 (Calcd for $C_{21}H_{22}BrNNaO_4S$ [M+Na]$^+$: 486.0351, 488.0330).

5-Methoxy-2-(2-methyl-4-oxopentan-2-yl)-1-tosylindolin-3-one (3df)

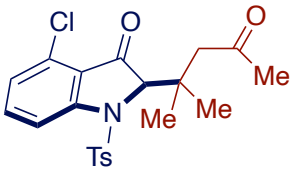


3df

126.7 mg, 61% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.92 (d, *J* = 9.2 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.24 (dd, *J* = 9.2, 2.9 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 2H), 6.86 (d, *J* = 2.9 Hz, 1H), 4.60 (s, 1H), 3.78 (s, 3H), 2.93 (d, *J* = 18.3 Hz, 1H), 2.56 (d, *J* = 18.3 Hz, 1H), 2.30 (s, 3H), 2.19 (s, 3H), 1.02 (s, 3H), 0.95 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 207.7, 200.2, 158.1, 148.6, 144.7, 131.7, 129.8, 129.7, 127.9, 125.4, 121.9, 104.4, 71.8, 55.8, 51.6,

38.1, 31.2, 25.4, 22.9, 21.6; HRMS (ESI) *m/z*: 438.1351 (Calcd for $C_{22}H_{25}NNaO_5S$ $[M+Na]^+$: 438.1351).

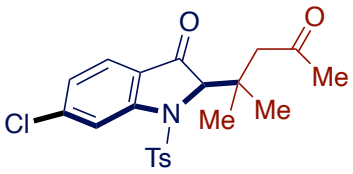
4-Chloro-2-(2-methyl-4-oxopentan-2-yl)-1-tosylindolin-3-one (3ff)



3ff

146.6 mg, 70% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 9.2 Hz, 1H), 7.54 (t, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.73 (s, 1H), 2.84 (d, *J* = 18.3 Hz, 1H), 2.64 (d, *J* = 18.9 Hz, 1H), 2.33 (s, 3H), 2.19 (s, 3H), 1.05 (s, 3H), 0.98 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 207.6, 197.1, 155.9, 145.3, 136.5, 132.0, 131.3, 130.0, 127.8, 127.5, 124.7, 118.8, 71.3, 51.2, 38.3, 31.2, 25.6, 23.1, 21.7; HRMS (ESI) *m/z*: 442.0855, 444.0829 (Calcd for $C_{21}H_{22}ClNNaO_4S$ $[M+Na]^+$: 442.0856, 444.0826).

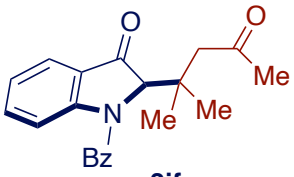
6-Chloro-2-(2-methyl-4-oxopentan-2-yl)-1-tosylindolin-3-one (3gf)



3gf

114.1 mg, 54% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.05 (d, *J* = 1.7 Hz, 1H), 7.38 (d, *J* = 8.6 Hz, 1H), 7.34 (d, *J* = 8.6 Hz, 2H), 7.20 (d, *J* = 8.0, 1.7 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.70 (s, 1H), 2.90 (d, *J* = 18.9 Hz, 1H), 2.57 (d, *J* = 18.9 Hz, 1H), 2.31 (s, 3H), 2.19 (s, 3H), 1.01 (s, 3H), 0.97 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 207.7, 198.5, 155.2, 145.2, 143.0, 131.9, 130.0, 127.8, 127.0, 126.8, 124.4, 120.7, 71.5, 51.4, 38.2, 31.2, 25.4, 22.9, 21.7; HRMS (ESI) *m/z*: 442.0857, 444.0824 (Calcd for $C_{21}H_{22}ClNNaO_4S$ $[M+Na]^+$: 442.0856, 444.0826).

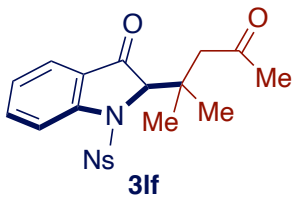
1-Benzoyl-2-(2-methyl-4-oxopentan-2-yl)indolin-3-one (3jf)



3jf

100.1 mg, 60% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.66 (d, *J* = 8.0 Hz, 1H), 7.58–7.63 (m, 3H), 7.52 (t, *J* = 7.5 Hz, 2H), 7.34 (td, *J* = 8.0, 1.2 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 6.88 (d, *J* = 7.5 Hz, 1H), 5.31 (s, 1H), 2.83 (d, *J* = 17.8 Hz, 1H), 2.60 (d, *J* = 17.8 Hz, 1H), 2.14 (s, 3H), 1.10 (s, 3H), 0.95 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 207.3, 199.7, 170.9, 154.0, 136.4, 136.4, 131.9, 129.1, 128.5, 126.3, 124.0, 123.8, 116.4, 69.5, 50.5, 39.6, 31.8, 26.0, 23.3; HRMS (ESI) *m/z*: 358.1419 (Calcd for $C_{21}H_{21}NNaO_3$ $[M+Na]^+$: 358.1419).

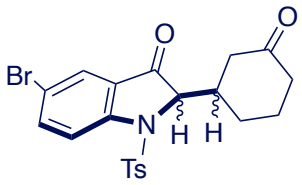
2-(2-Methyl-4-oxopentan-2-yl)-1-((4-nitrophenyl)sulfonyl)indolin-3-one (3lf)



3lf

78.8 mg, 38% yield. colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.80 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.62–7.66 (m, 2H), 7.57 (d, *J* = 6.9 Hz, 1H), 7.56 (td, *J* = 8.1, 1.8 Hz, 1H), 7.47 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.28 (d, *J* = 7.5 Hz, 1H), 4.85 (s, 1H), 2.81 (d, *J* = 18.4 Hz, 1H), 2.65 (d, *J* = 18.4 Hz, 1H), 2.18 (s, 3H), 1.07 (s, 3H), 1.00 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 207.5, 198.9, 152.6, 148.6, 136.7, 135.0, 132.2, 131.5, 129.2, 128.3, 126.4, 124.4, 123.9, 119.6, 72.9, 51.0, 38.7, 31.6, 25.2, 23.0; HRMS (ESI) *m/z*: 439.0944 (Calcd for $C_{20}H_{20}N_2NaO_6S$ $[M+Na]^+$: 439.0940).

5-Bromo-2-(3-oxocyclohexyl)-1-tosylindolin-3-one (3ca')



3ca'

83.9 mg, 36% yield (dr = 1:1). colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (d, *J* = 9.2 Hz, 1/2H), 7.94 (d, *J* = 9.2 Hz, 1/2H), 7.76 (d, *J* = 9.2 Hz, 1H), 7.65-7.68 (m, 1H), 7.52 (d, *J* = 8.6 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.19-7.23 (m, 2H), 3.91 (d, *J* = 3.5 Hz, 1/2H), 3.81 (d, *J* = 2.9 Hz, 1/2H), 2.78-2.81 (m, 1H), 2.67-2.74 (m, 1/2H), 2.36 (s, 3H), 2.32-2.48 (m, 2H), 2.18-2.26 (m, 3/2H), 2.01-2.09 (m, 1H), 1.88-1.96 (m, 1H), 1.73 (m, 1/2H), 1.56-1.65 (m, 1H), 1.35-1.42 (m, 1/2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 209.5, 209.3, 196.9, 196.8, 152.7, 152.6, 145.7, 145.6, 140.1, 132.6, 132.5, 130.3, 130.2, 127.7, 127.5, 127.4, 127.3, 126.9, 126.8, 119.9, 119.5, 118.9, 118.7, 70.5, 70.0, 43.2, 42.7, 42.5, 42.3, 41.2, 41.0, 25.9, 25.7, 24.7, 21.7; HRMS (ESI) *m/z*: 484.0199, 486.0176 (Calcd for $C_{21}H_{20}BrNNaO_4S$ $[M+Na]^+$: 484.0194, 486.0174).

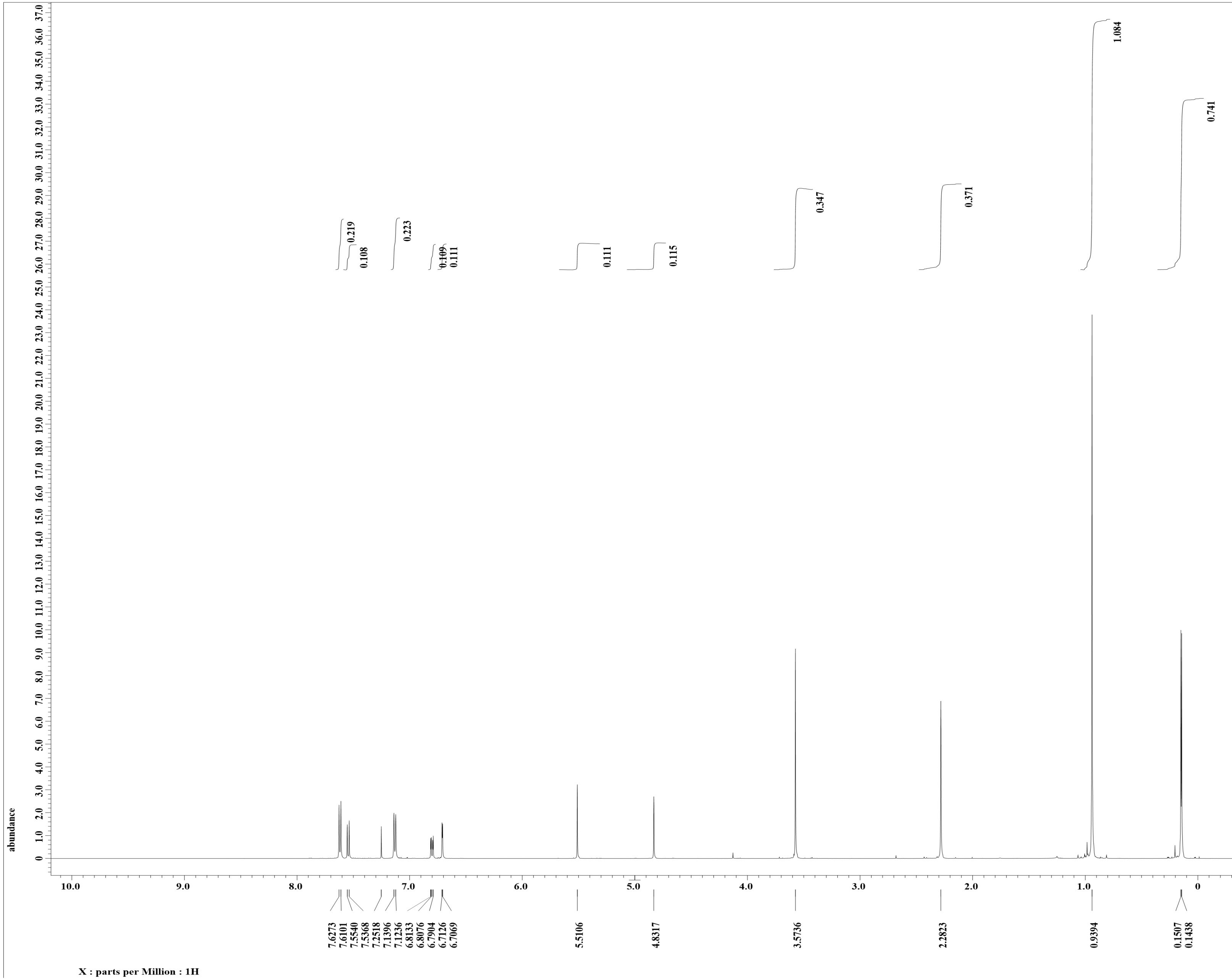
3. Supplementary References

(S1) Hodson, H. F.; Madge, D. J.; Slawin, A. N. Z.; Widdowson, D. A.; Williams, D. J. *Tetrahedron* **1994**, *50*, 1899.

(S2) Abe, T.; Kosaka, Y.; Kawasaki, T.; Ohata, Y.; Yamada, K. *Chem. Pharm Bull.*, **2020**, *68*, 555–558

(S3) Hirao, S.; Yamashiro, T.; Kohira, K.; Mishima, N.; Abe, T. *Chem. Commun.* **2020**, *56,* 5139–5142.

(S4) Zefirova, O. N.; Baranova, T. Y.; Ivanova, A. A.; Ivanov, A. A.; Zefirov, N. S. *Bioorg. Chem.* **2011**, *39*, 67.

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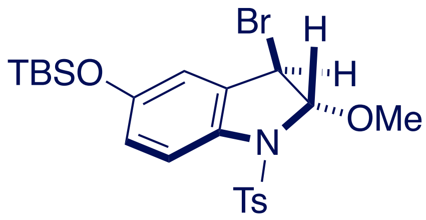
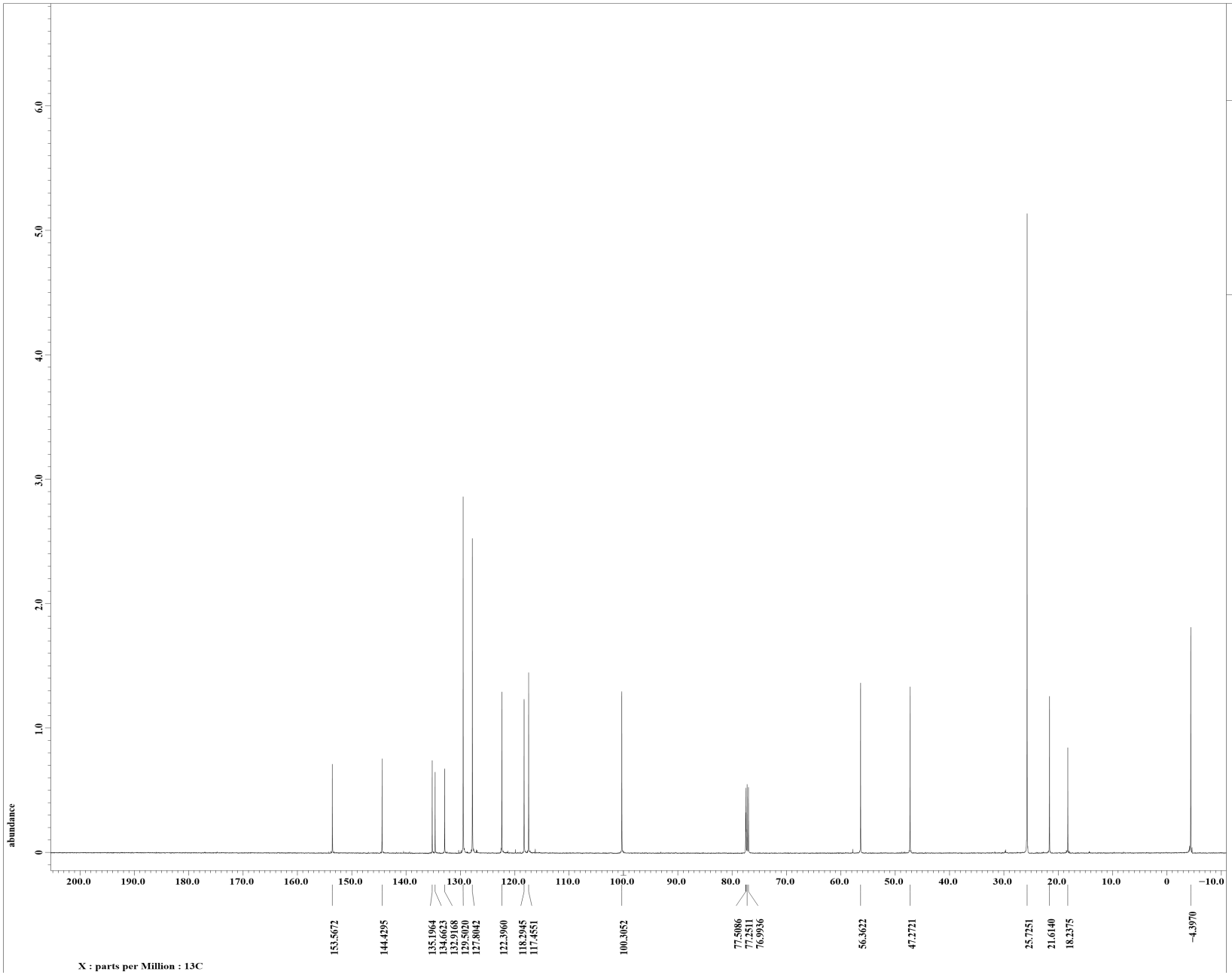


B-5

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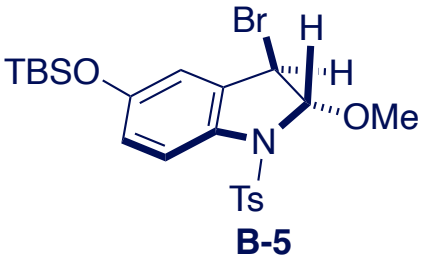
Current_time      = 30-MAR-2020 12:17:49

Comment           = 5-TBSO-ROBIN
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             = 1790
Total_scans       = 1790

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          = 24.1[dC]
```

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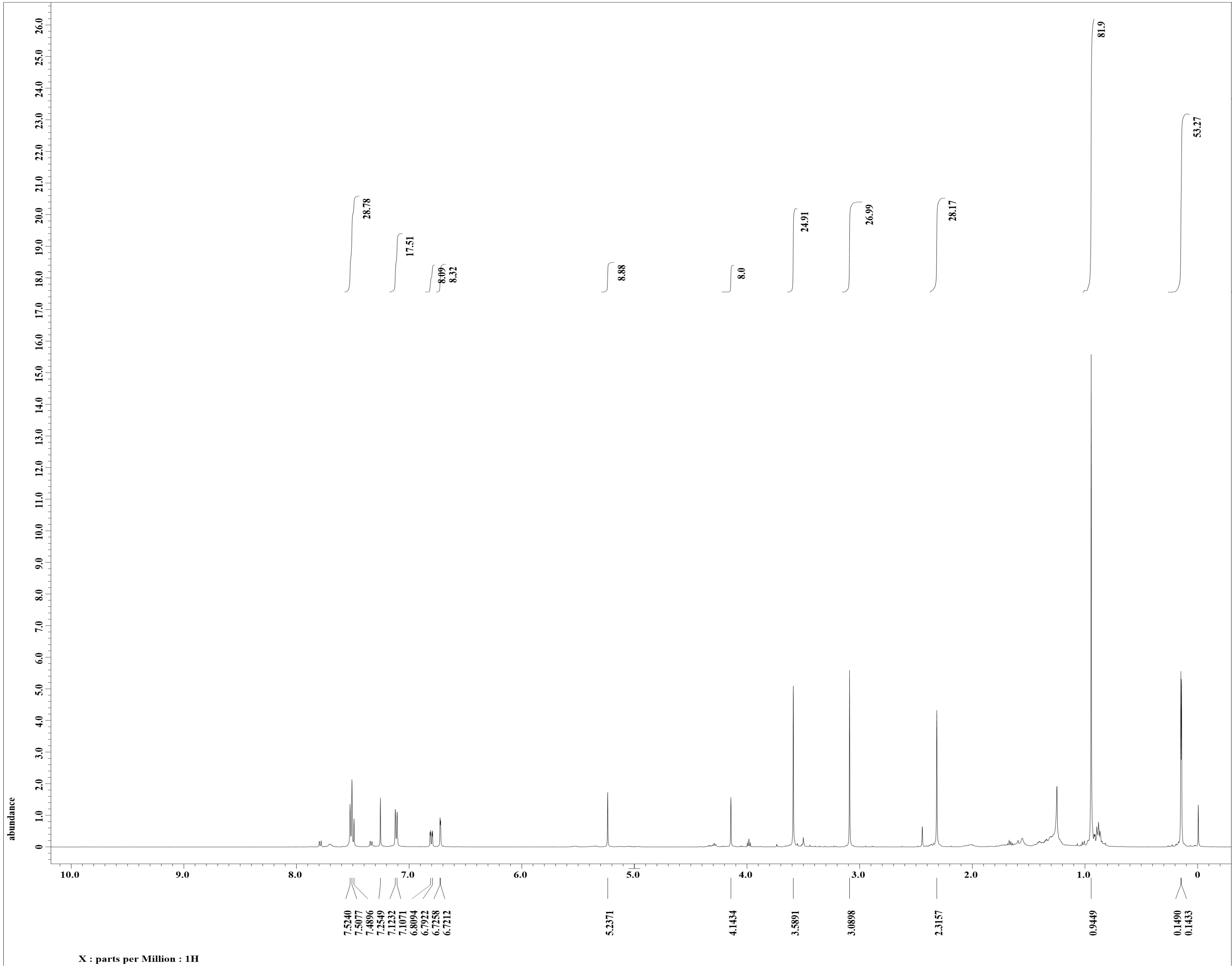



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

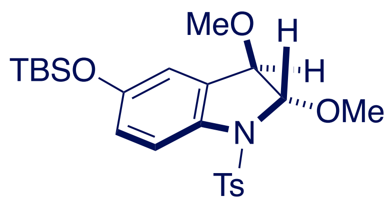
Derived from: TA2020-0330-14.jdf
```

```
Filename          = TA2020-0330-17.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#615601
Solvent           = CHLOROFORM-D
Creation_time     = 15-JUN-2000 18:52:29
Revision_time     = 30-MAR-2020 17:10:14
Current_time      = 30-MAR-2020 17:10:56

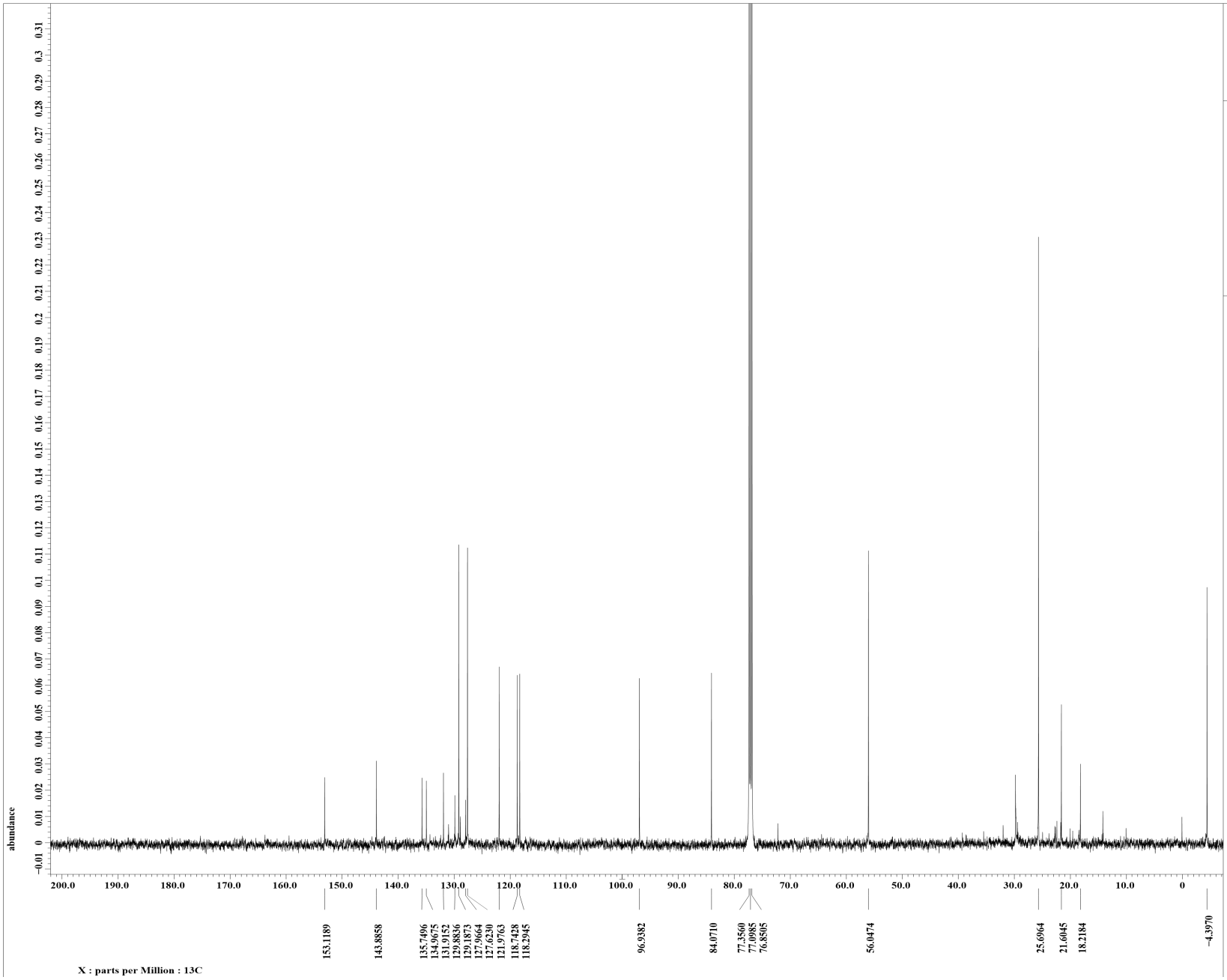
Comment           = DiMeOIN(5-TBSO)
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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          = 22.9[dC]
```



1e



---- 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

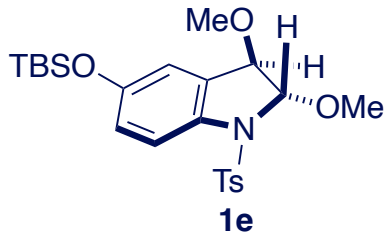
Derived from: TA2020-0330-17.jdf

Filename = TA2020-0330-18.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#616444
Solvent = CHLOROFORM-D
Creation_time = 15-JUN-2000 21:42:07
Revision_time = 15-APR-2020 19:39:09
Current_time = 15-APR-2020 19:39:57

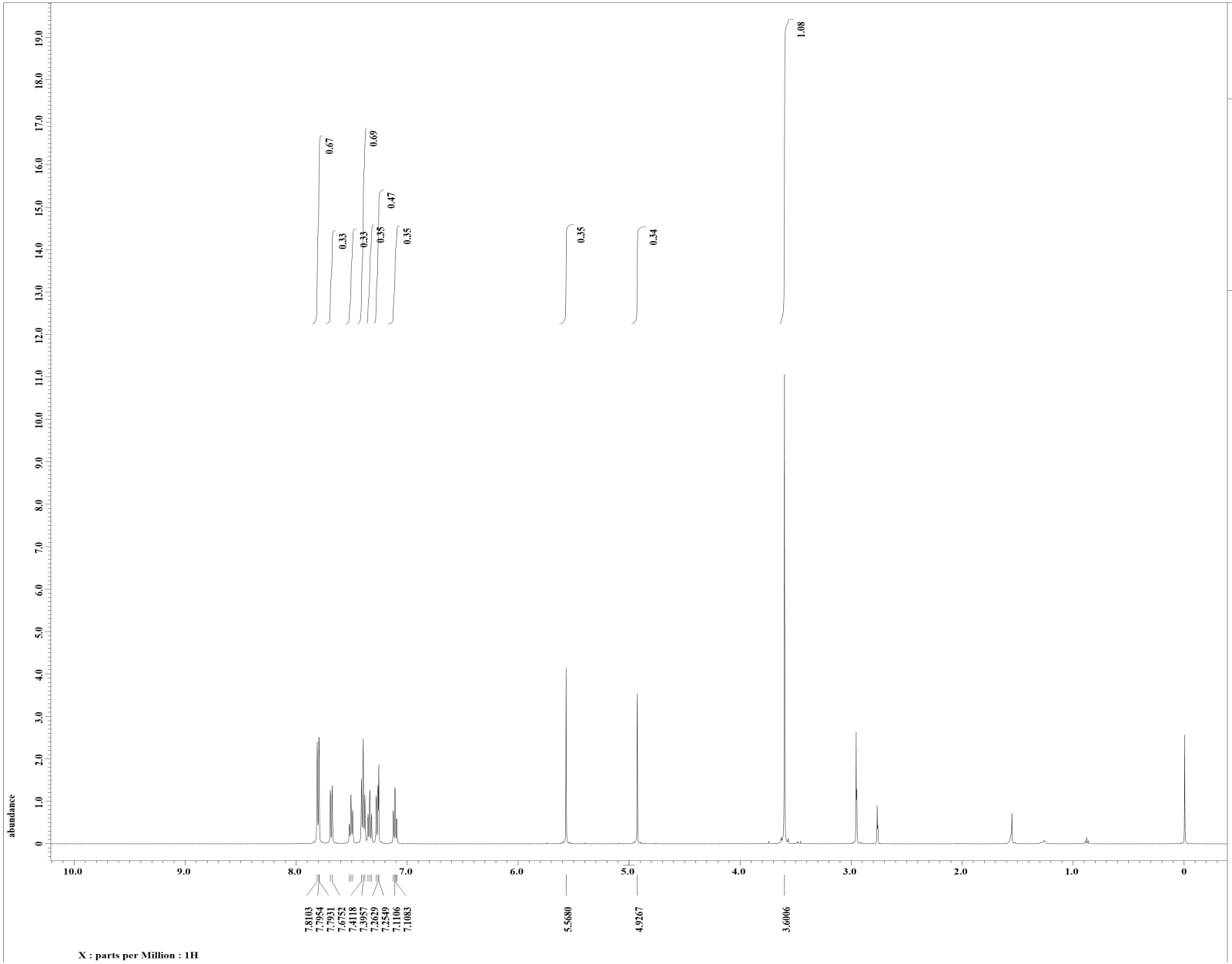
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA500
Spectrometer = DELTA2_NMR

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 = 3571
Total_scans = 3571

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 = 23.2[dC]



1e



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

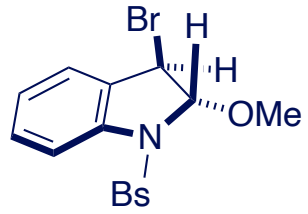
Derived from: Bs-ROBIN-1H-1.jdf
```

```
Filename          = Bs-ROBIN-1H-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#6763I3
Solvent           = CHLOROFORM-D
Creation_time     = 24-JUN-2000 20:33:23
Revision_time     =  8-APR-2020 18:49:54
Current_time      =  8-APR-2020 18:50:35

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          = 23.5[dC]
```



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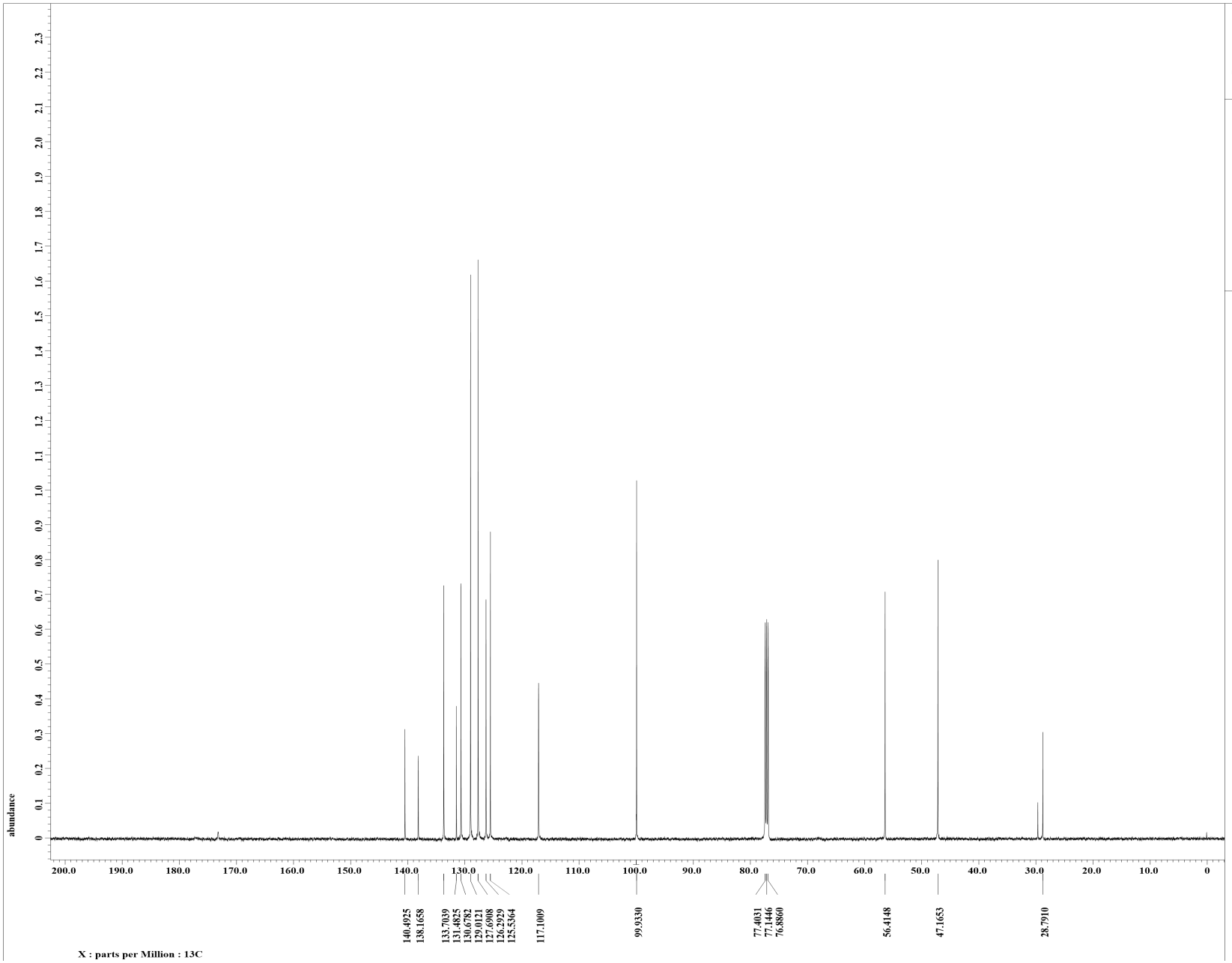



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

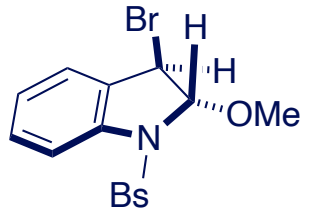
Derived from: TA200408-4.jdf
```

```
Filename          = TA200408-6.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#607750
Solvent           = CHLOROFORM-D
Creation_time     =  8-APR-2020 18:22:53
Revision_time     =  8-APR-2020 19:00:34
Current_time      =  8-APR-2020 19:01:18

Content           = Bs-ROBIN-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             = 2666
Total_scans       = 2666

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]
```



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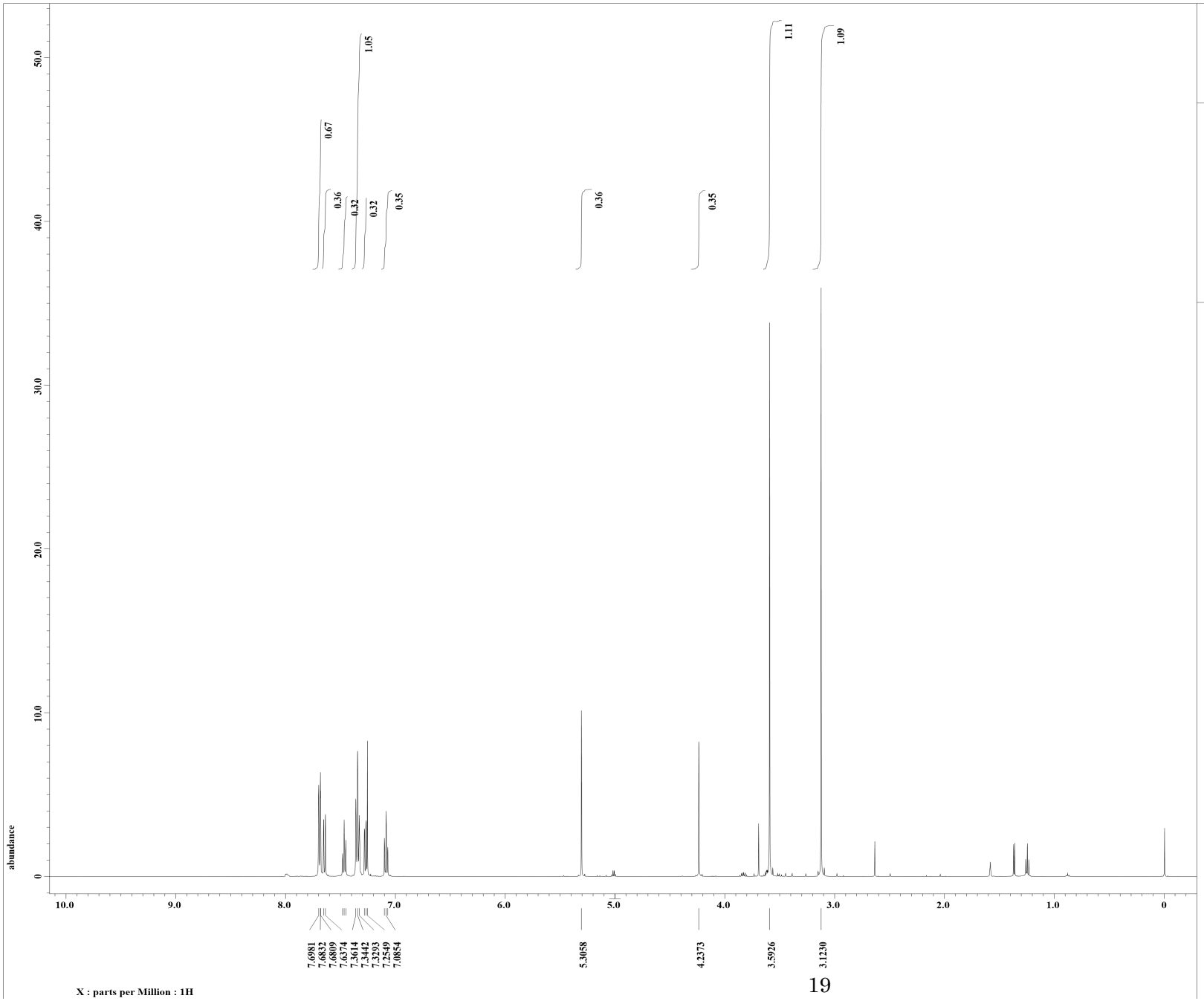


```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

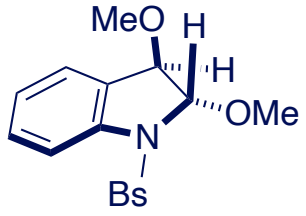
Derived from: Bs-DiMeOIN-1.jdf
```

```
Filename          = Bs-DiMeOIN-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#644967
Solvent           = CHLOROFORM-D
Creation_time     = 26-JUN-2000 19:41:04
Revision_time     = 10-APR-2020 17:59:35
Current_time      = 10-APR-2020 18:00:51

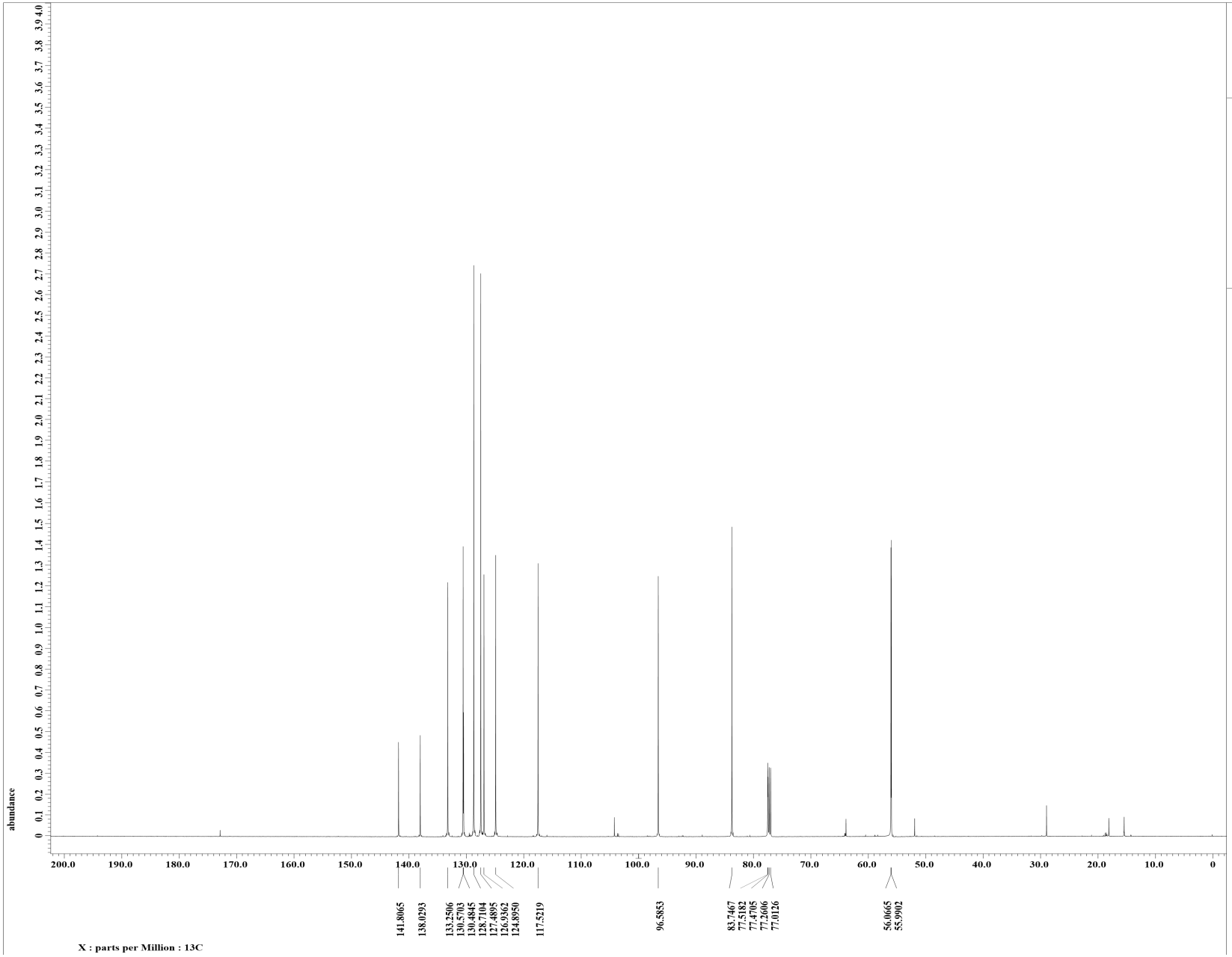
Comment           = Bs-DiMeOIN
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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          = 22.4[dC]
```



1k




```
---- 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

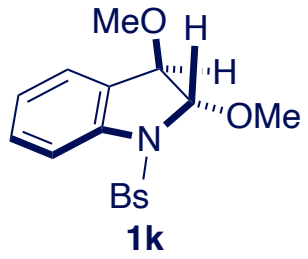
Derived from: Bs-DiMeOIN-2.jdf
```

```
Filename            = Bs-DiMeOIN-5.jdf
Author              = delta
Experiment          = single_pulse_dec
Sample_id           = S#647870
Solvent             = CHLOROFORM-D
Creation_time       = 27-JUN-2000 16:19:23
Revision_time       = 11-APR-2020 14:36:10
Current_time        = 11-APR-2020 14:37:12

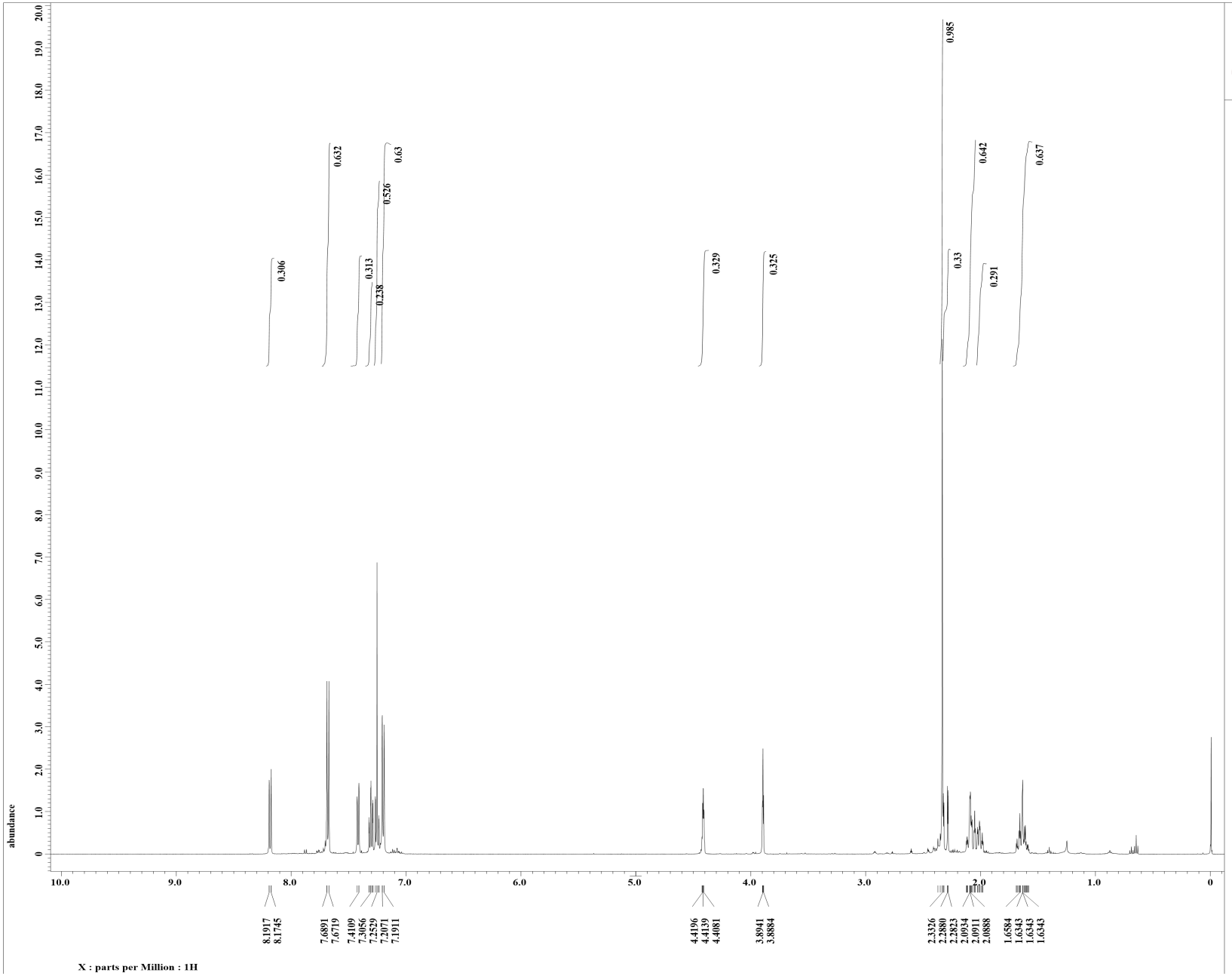
Comment             = Bs-DiMeOIN
Data_format         = 1D COMPLEX
Dim_size            = 26214
Dim_title           = 13C
Dim_units           = [ppm]
Dimensions          = X
Site                = ECA500
Spectrometer        = DELTA2_NMR

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               = 26126
Total_scans         = 26126

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            = 23.8[dC]
```



1k

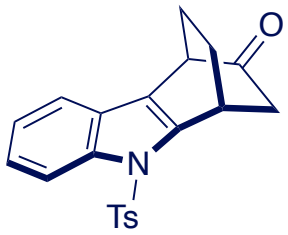


Filename = TA200316-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#571541
Solvent = CHLOROFORM-D
Creation_time = 16-MAR-2020 14:51:58
Revision_time = 16-MAR-2020 16:03:30
Current_time = 16-MAR-2020 16:03:47

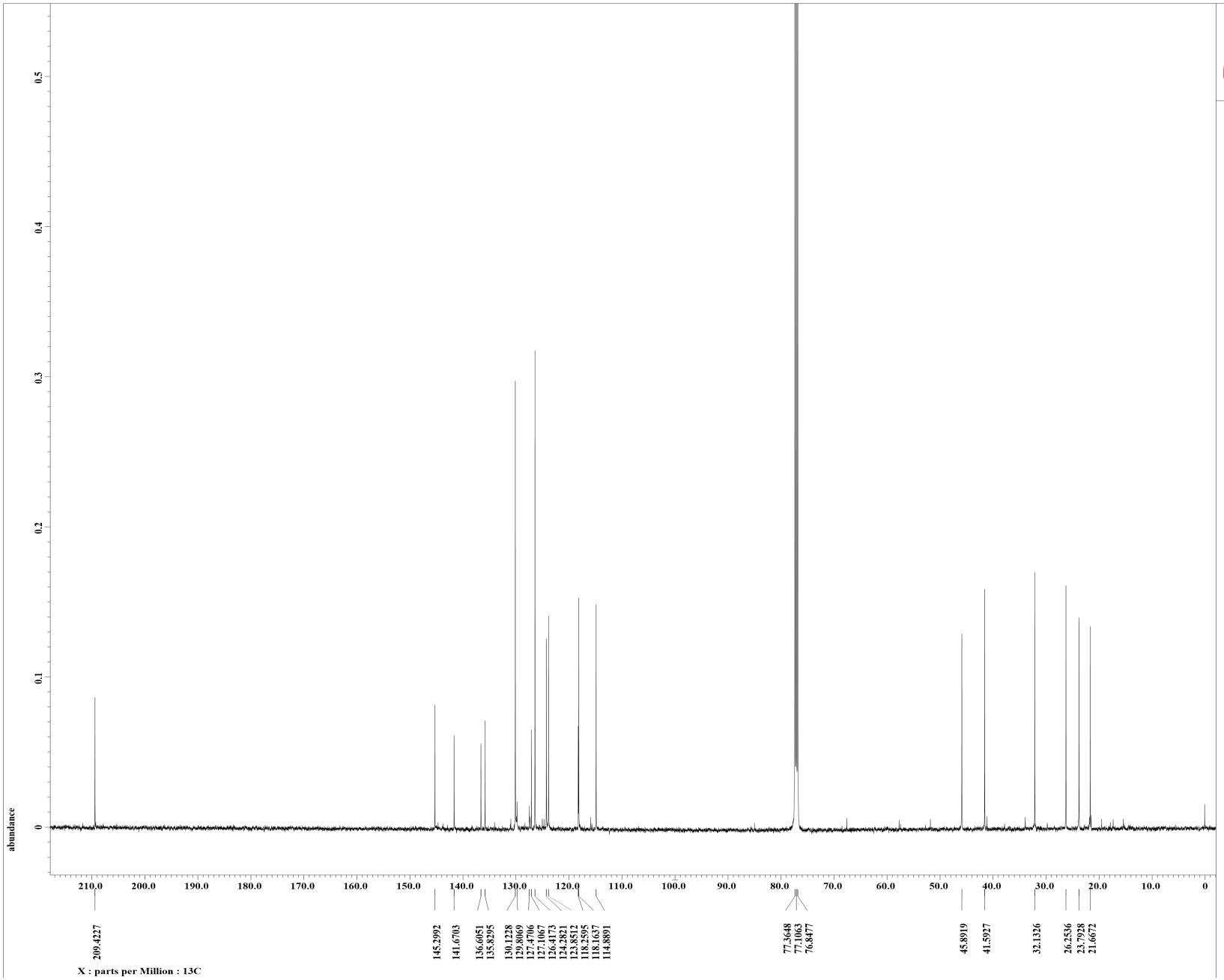
Content = R=H-cyclohexenone
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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 = 23.2[dC]



3aa



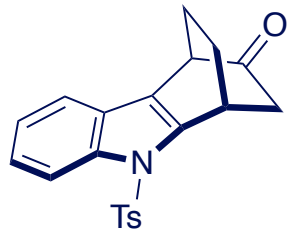
JEOL

```
Filename          = TA200316-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#572819
Solvent           = CHLOROFORM-D
Creation_time     = 17-MAR-2020 07:42:41
Revision_time     = 17-MAR-2020 08:45:34
Current_time      = 17-MAR-2020 08:46:10

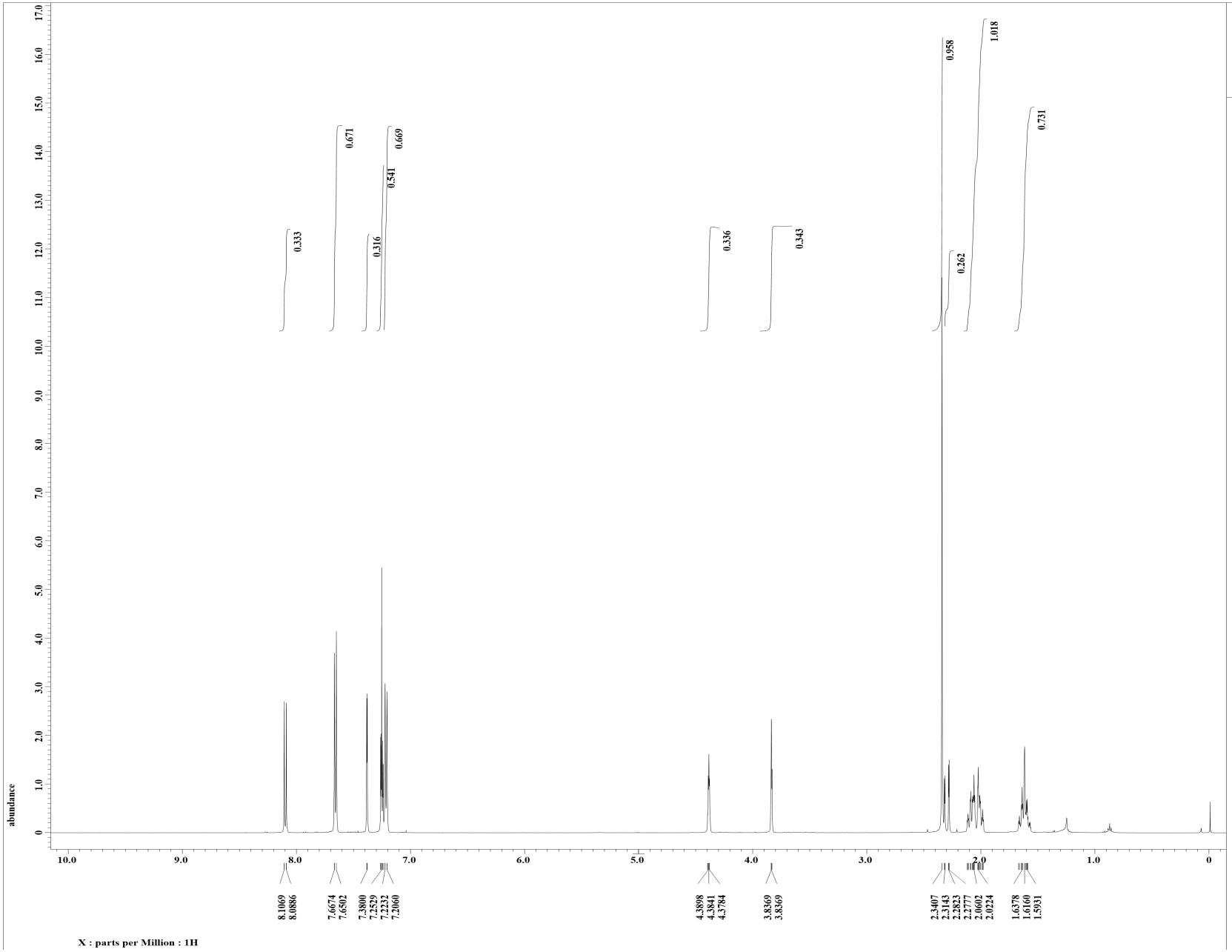
Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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           = TRUE
Mod_return        = 1
Scans             = 21329.0
Total_scans       = 21329.0

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          = 23.9[dC]
```



3aa

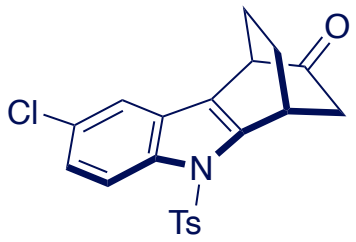


Filename = TA200318-6.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#495478
Solvent = CHLOROFORM-D
Creation_time = 18-MAR-2020 12:53:52
Revision_time = 18-MAR-2020 13:50:10
Current_time = 18-MAR-2020 13:50:40

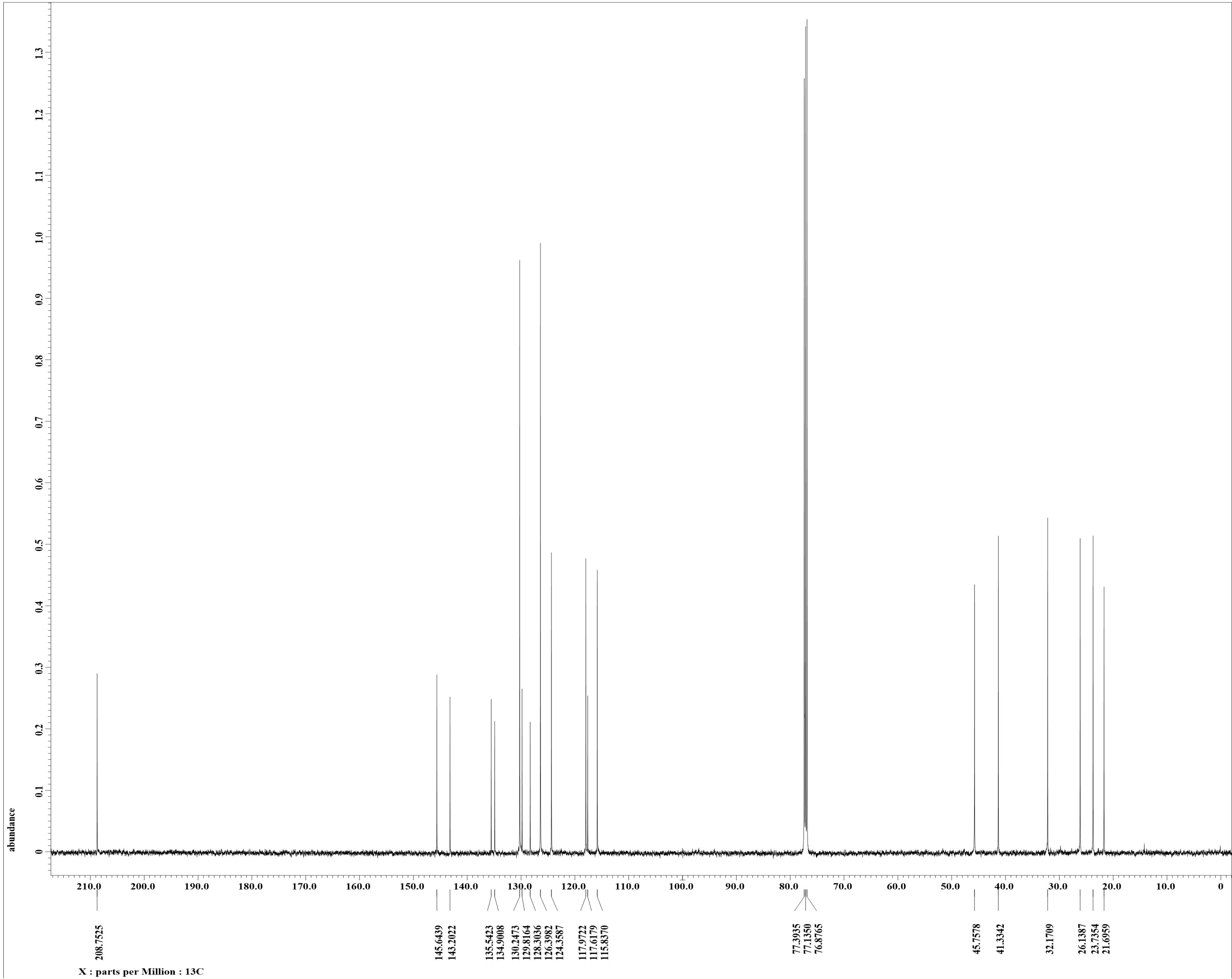
Content = 5Cl-cyclohexenone
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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 = 38
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 23.6[dC]



3ba



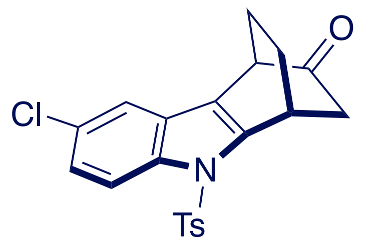
JEOL

```
Filename           = TA200318-8.jdf
Author             = delta
Experiment         = single_pulse_dec
Sample_id          = S#496811
Solvent            = CHLOROFORM-D
Creation_time      = 18-MAR-2020 14:44:35
Revision_time      = 18-MAR-2020 15:38:42
Current_time       = 18-MAR-2020 15:39:22

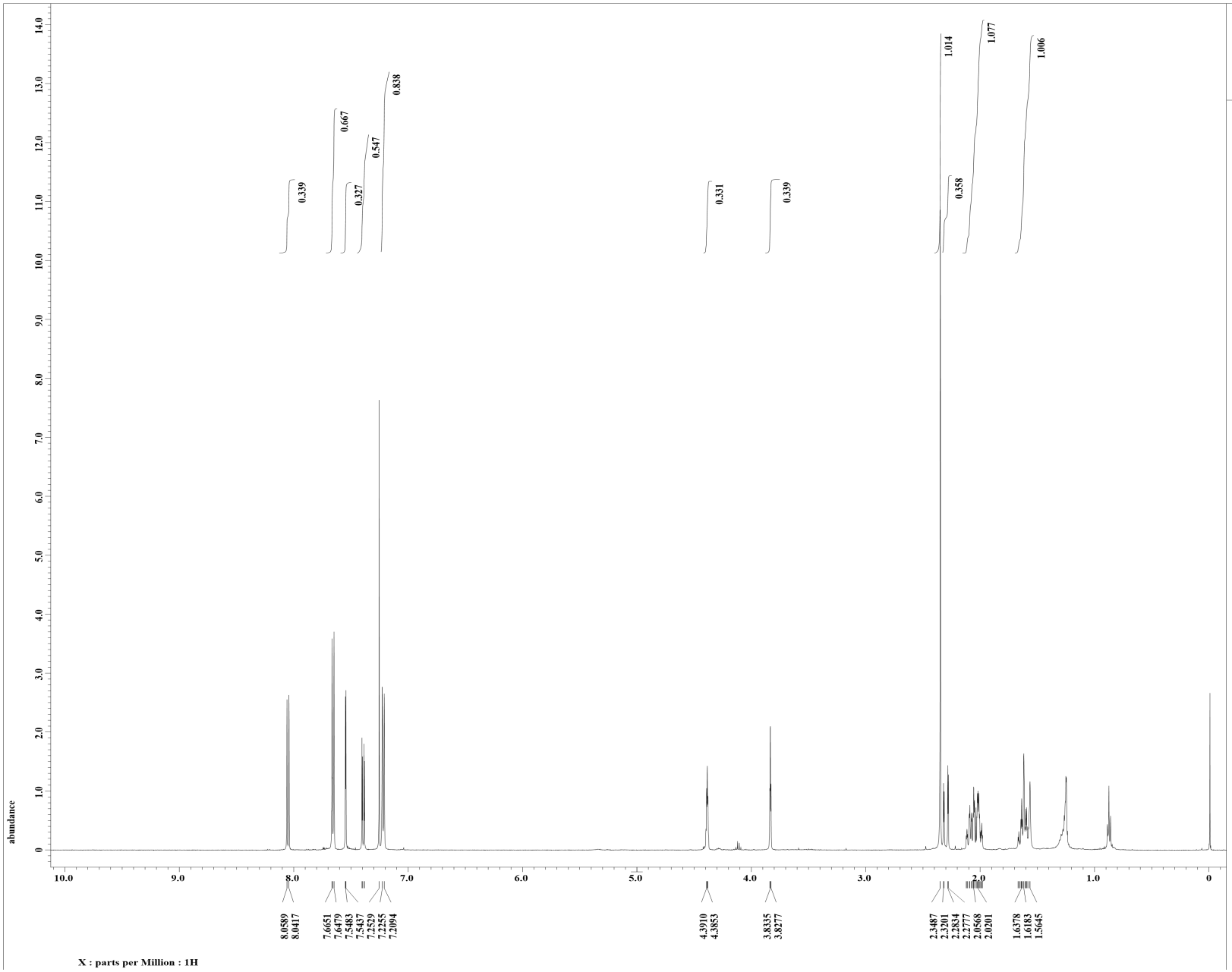
Content            = single pulse decouple
Data_format        = 1D COMPLEX
Dim_size           = 26214
Dim_title          = 13C
Dim_units          = [ppm]
Dimensions         = X
Site               = ECA 500
Spectrometer       = DELTA2_NMR

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              = 2311
Total_scans        = 2311

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]
```



3ba

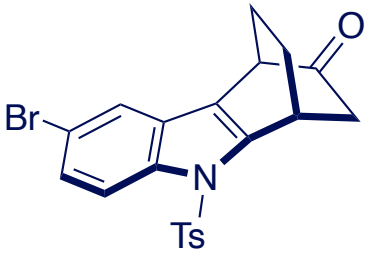


Filename = TA200319-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#628958
Solvent = CHLOROFORM-D
Creation_time = 19-MAR-2020 16:36:09
Revision_time = 19-MAR-2020 17:33:26
Current_time = 19-MAR-2020 17:33:55

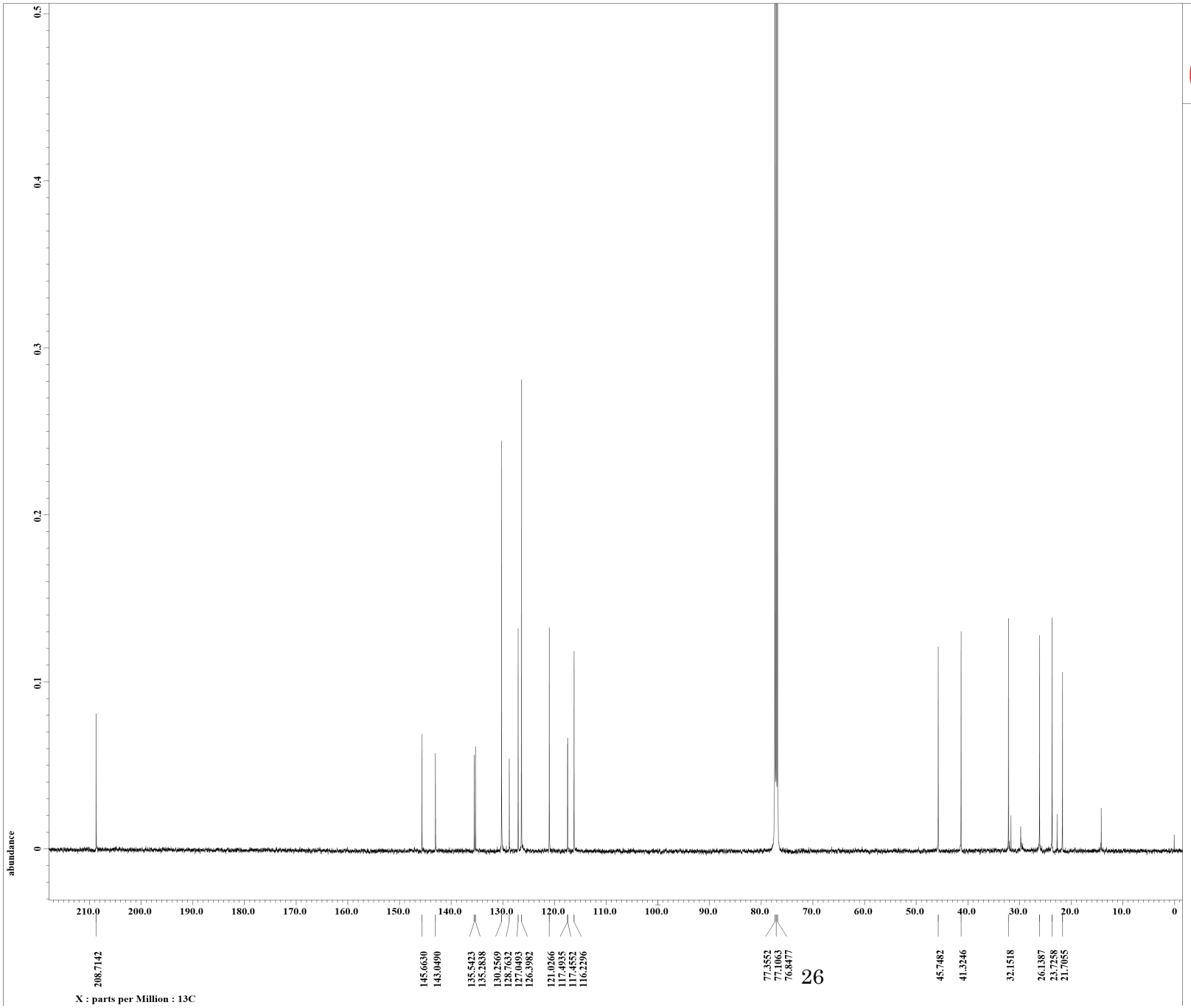
Content = rev-5Br
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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 = 23.5[dC]



3ca

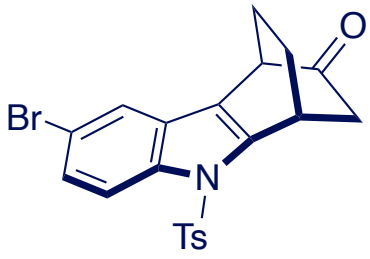


Filename = TA200319-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#630158
Solvent = CHLOROFORM-D
Creation_time = 20-MAR-2020 11:15:56
Revision_time = 20-MAR-2020 12:10:24
Current_time = 20-MAR-2020 12:11:28

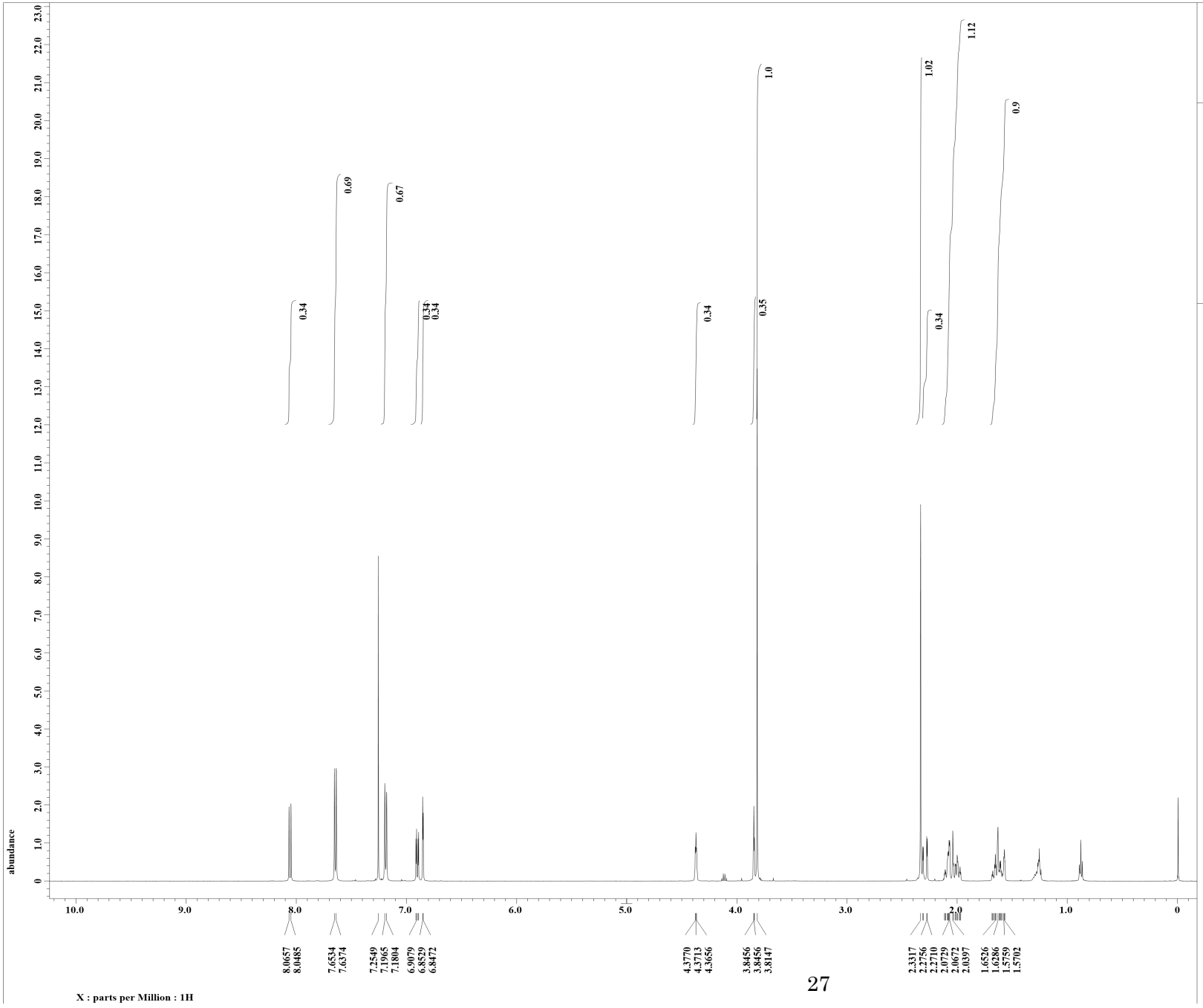
Content = rev-5Br
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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 = 23637
Total_scans = 23637

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
DecCoupling = 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 = 24.3[dC]



3ca




```
---- 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

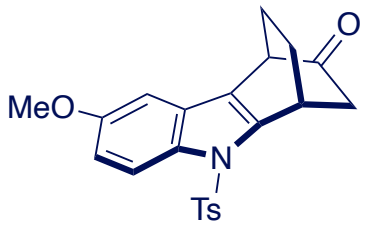
Derived from: TA2020-0323-5MeO-1.jdf
```

```
Filename          = TA2020-0323-5MeO-4.jd
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#574236
Solvent           = CHLOROFORM-D
Creation_time     =  8-JUN-2000 17:43:49
Revision_time     = 23-MAR-2020 16:07:20
Current_time      = 23-MAR-2020 16:07:53

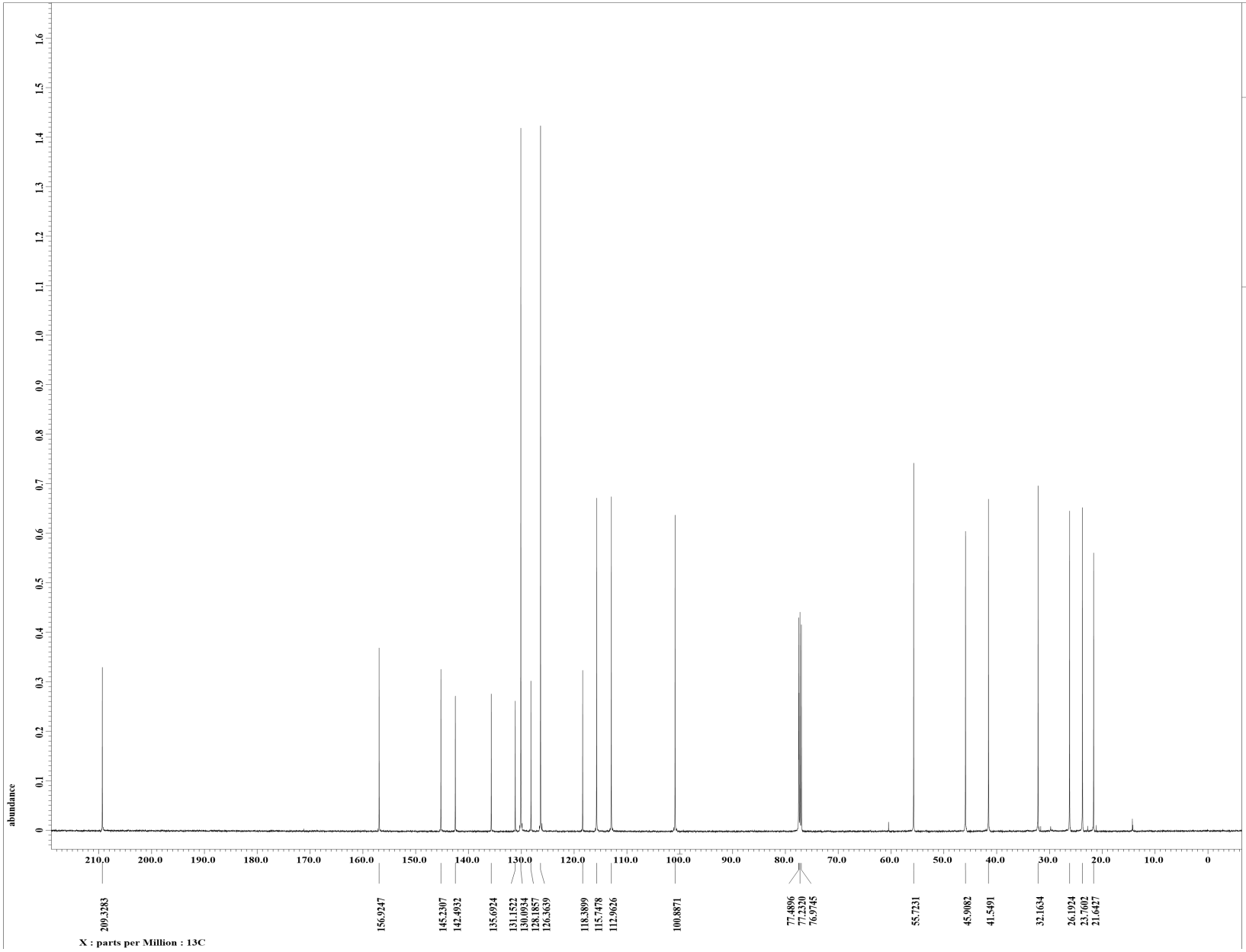
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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          = 22.7[dC]
```



3da




```
---- 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

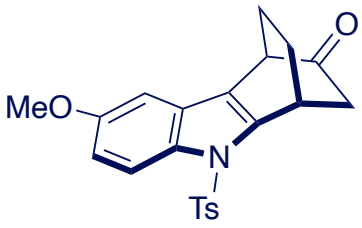
Derived from: TA2020-0323-5MeO-6.jdf
```

```
Filename          = TA2020-0323-5MeO-8.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#588990
Solvent           = CHLOROFORM-D
Creation_time     =  8-JUN-2000 20:54:33
Revision_time     = 23-MAR-2020 19:09:09
Current_time      = 23-MAR-2020 19:10:16

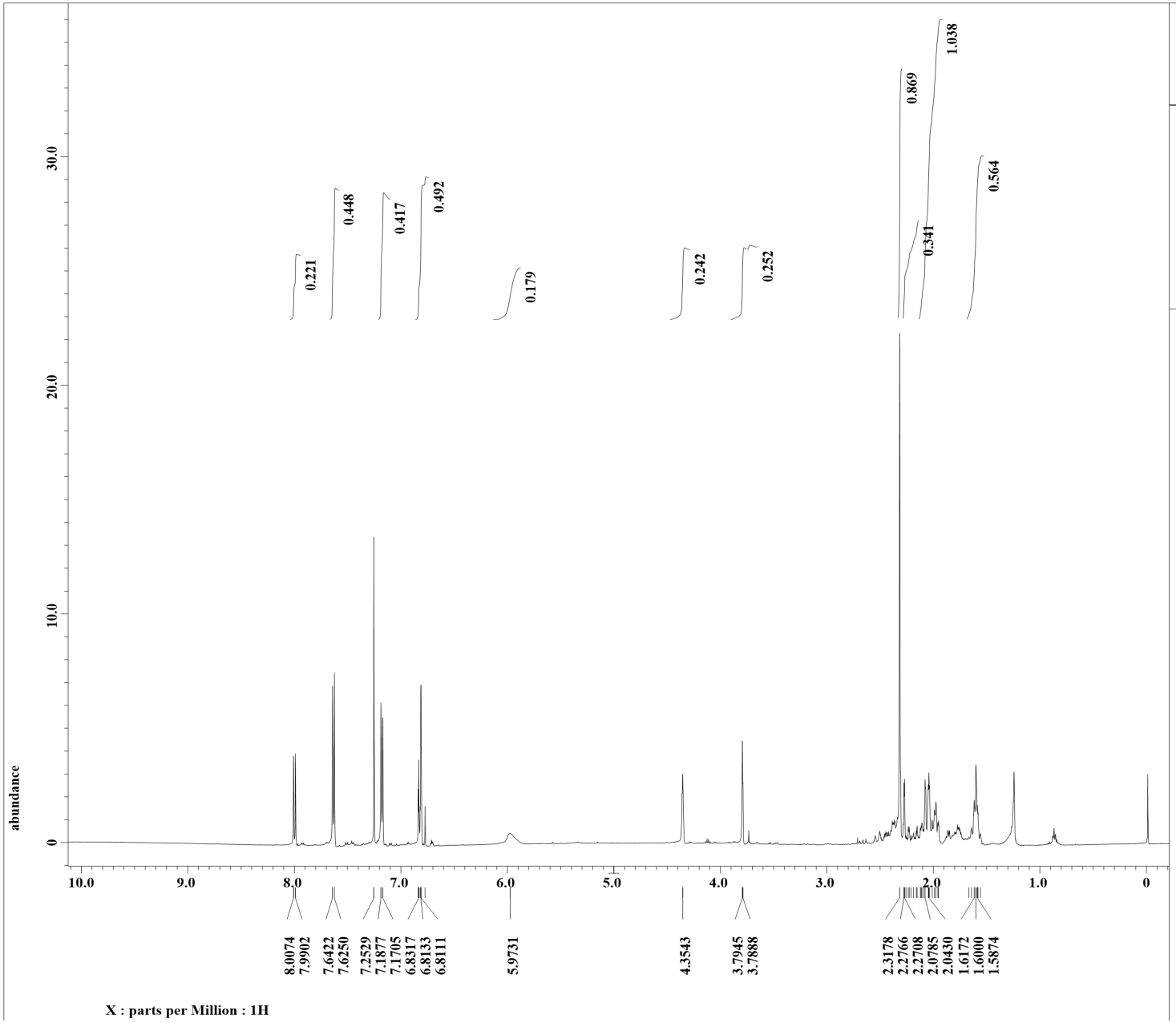
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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             = 3527
Total_scans       = 3527

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          = 23.6[dC]
```

3da



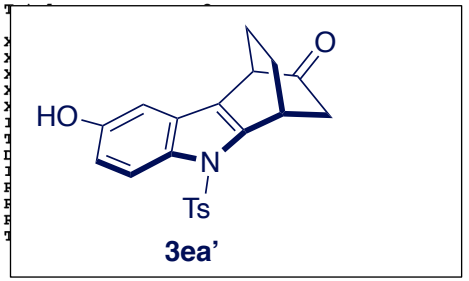
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA200402-1.jdf

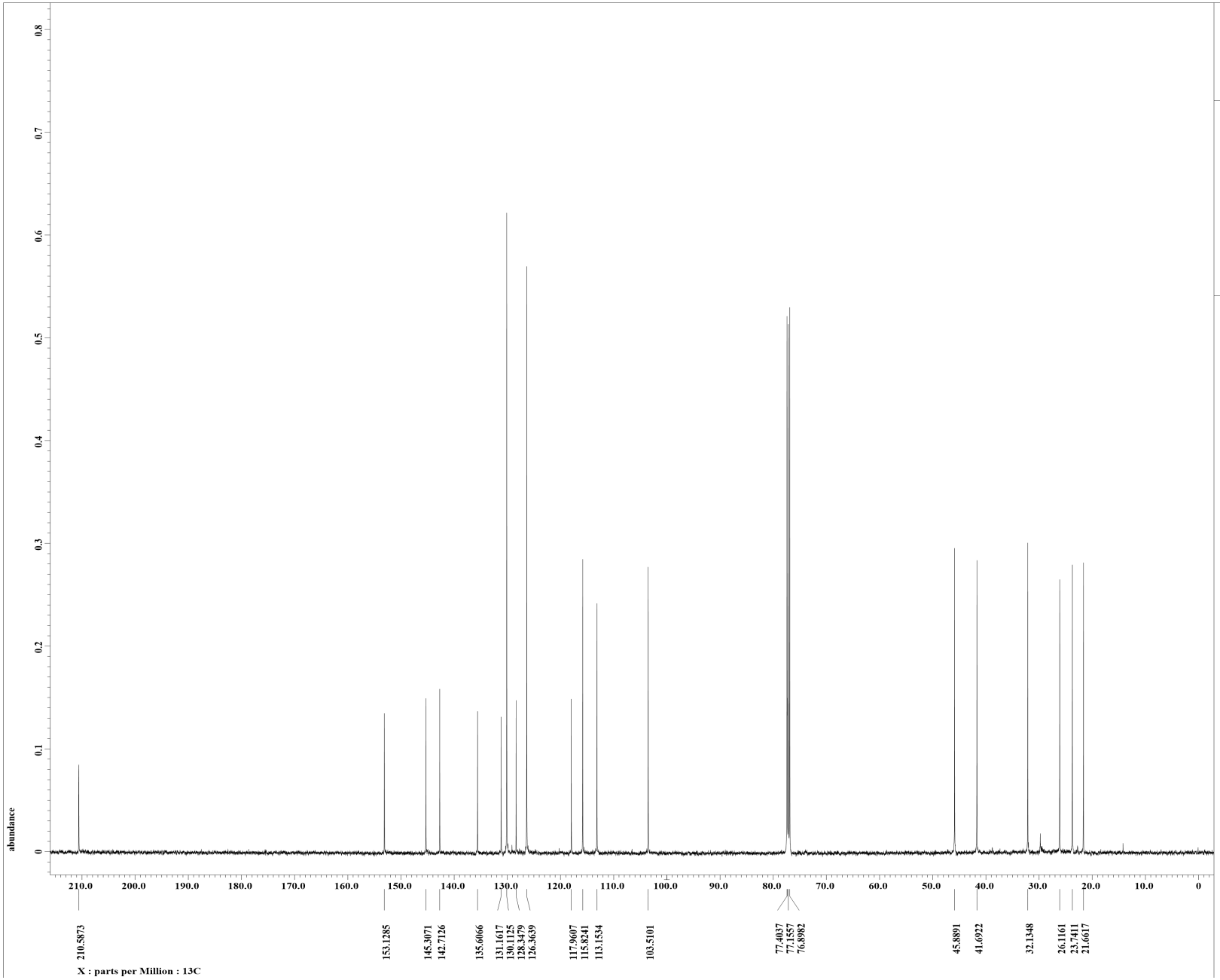
Filename = TA200402-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#425997
Solvent = CHLOROFORM-D
Creation_time = 3-APR-2020 11:14:50
Revision_time = 3-APR-2020 11:58:19
Current_time = 3-APR-2020 11:59:00

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 = TRUE
Mod_return = 1
Scans = 8



3ea'



```
----- 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

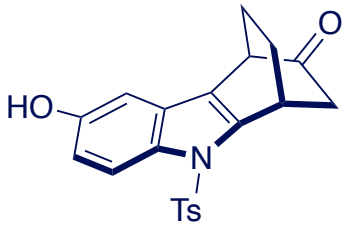
Derived from: TA2020-0404-2.jdf
```

```
Filename          = TA2020-0404-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#600995
Solvent           = CHLOROFORM-D
Creation_time     = 20-JUN-2000 20:27:59
Revision_time     =  4-APR-2020 18:43:00
Current_time      =  4-APR-2020 18:43:30

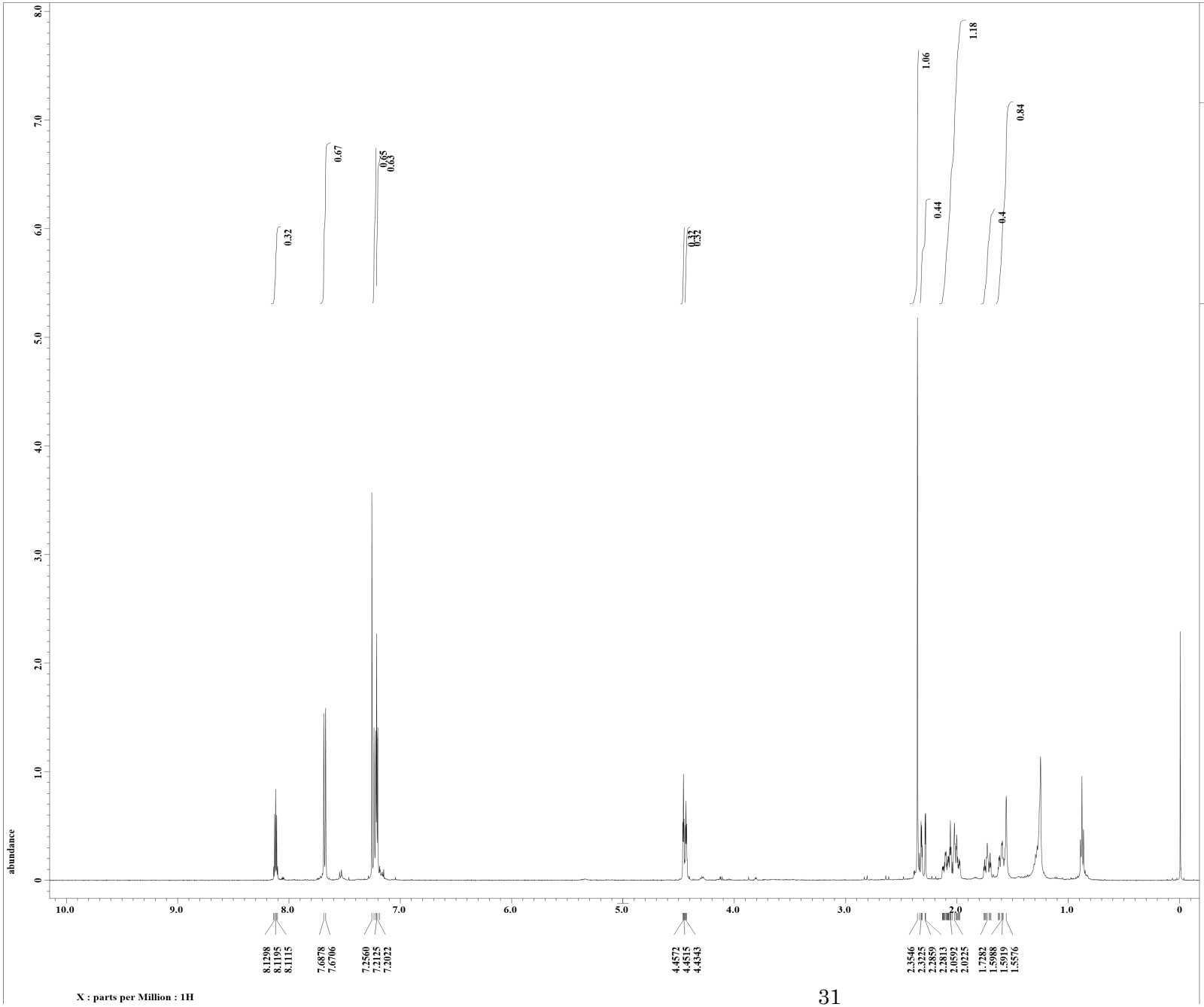
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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             = 2548
Total_scans       = 2548

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          = 23.9[dC]
```



3ea'



```
---- 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

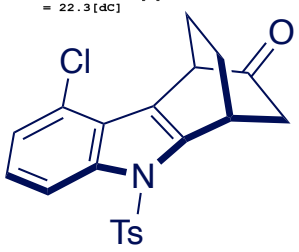
Derived from: TA2020-0319-4Cl2-4.jdf
```

```
Filename          = TA2020-0319-4Cl2-7.jd
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#576520
Solvent           = CHLOROFORM-D
Creation_time     =  4-JUN-2000 17:47:45
Revision_time     = 19-MAR-2020 16:05:28
Current_time      = 19-MAR-2020 16:06:10

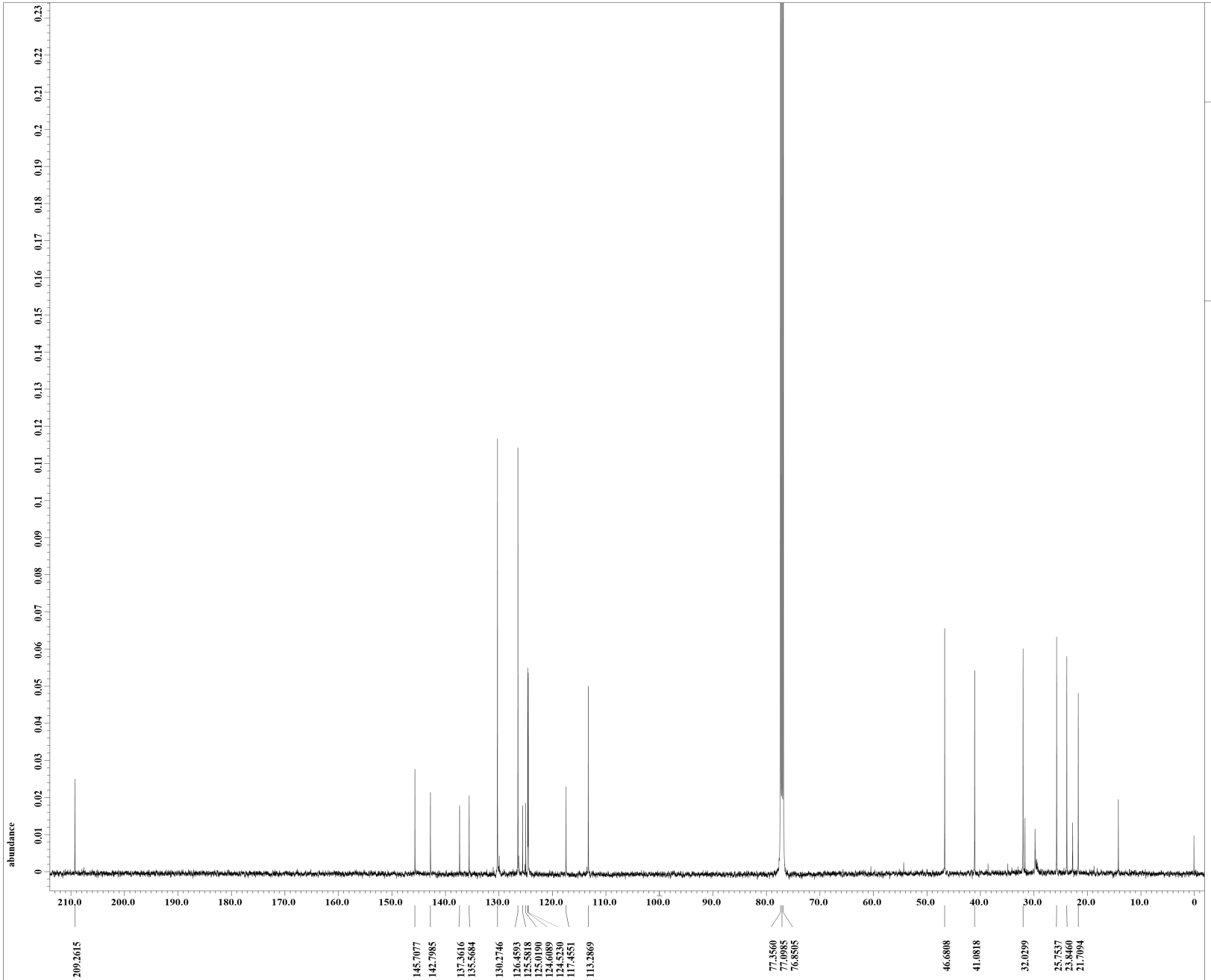
Comment           = 4Cl-cyclohexenone-2
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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]
```



3fa



```
---- 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

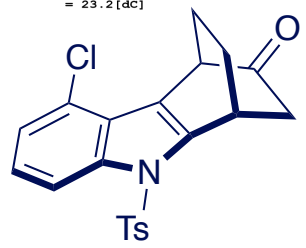
Derived from: TA2020-0319-4Cl2-5.jdf
```

```
Filename          = TA2020-0319-4Cl2-7.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#577220
Solvent           = CHLOROFORM-D
Creation_time     =  5-JUN-2000 13:23:13
Revision_time     = 20-MAR-2020 11:38:46
Current_time      = 20-MAR-2020 11:39:44

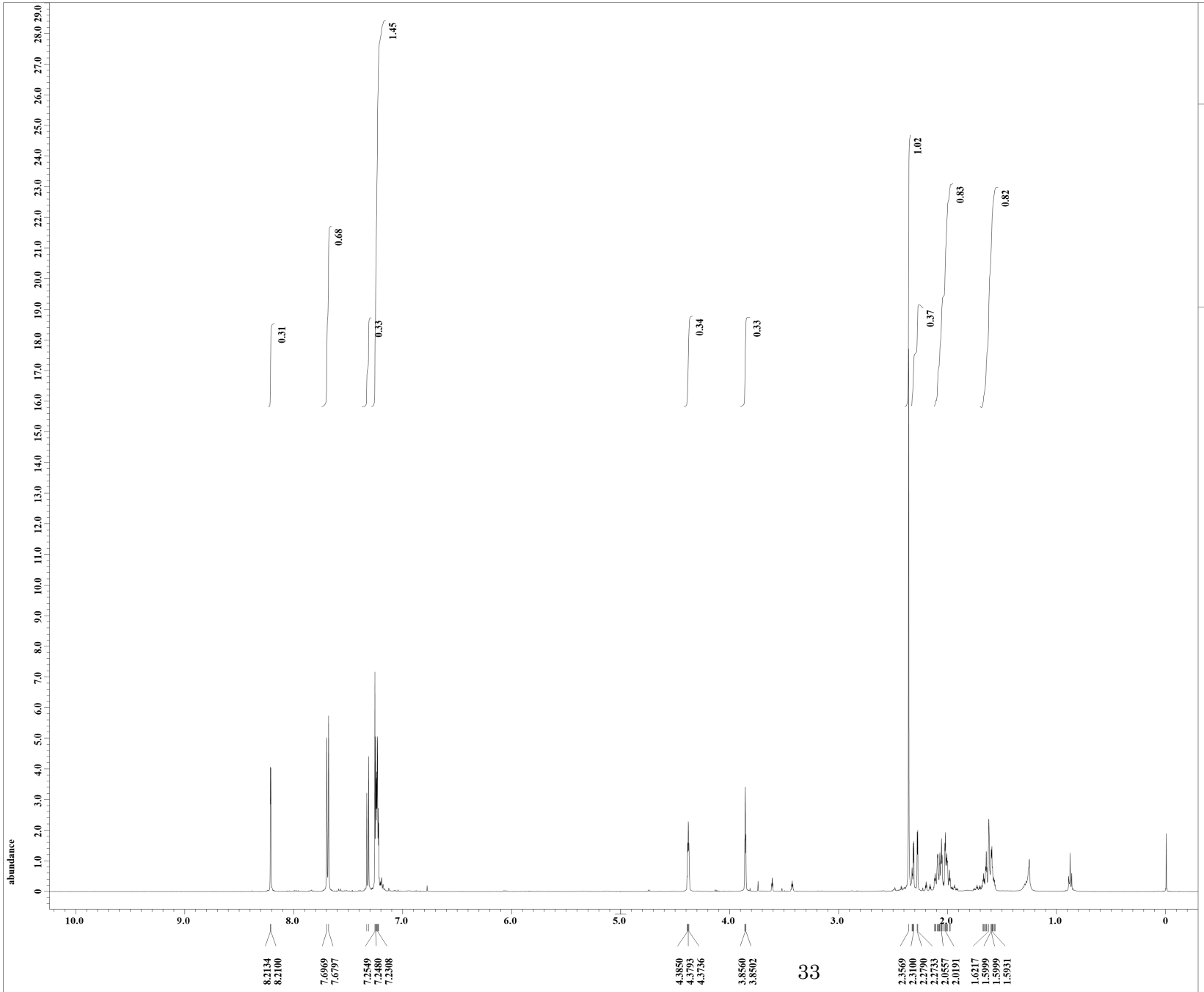
Comment           = 4Cl-cyclohexenone
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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             = 24875
Total_scans       = 24875

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          = 23.2[dC]
```



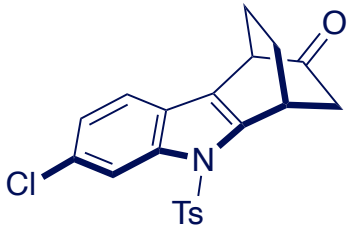
3fa



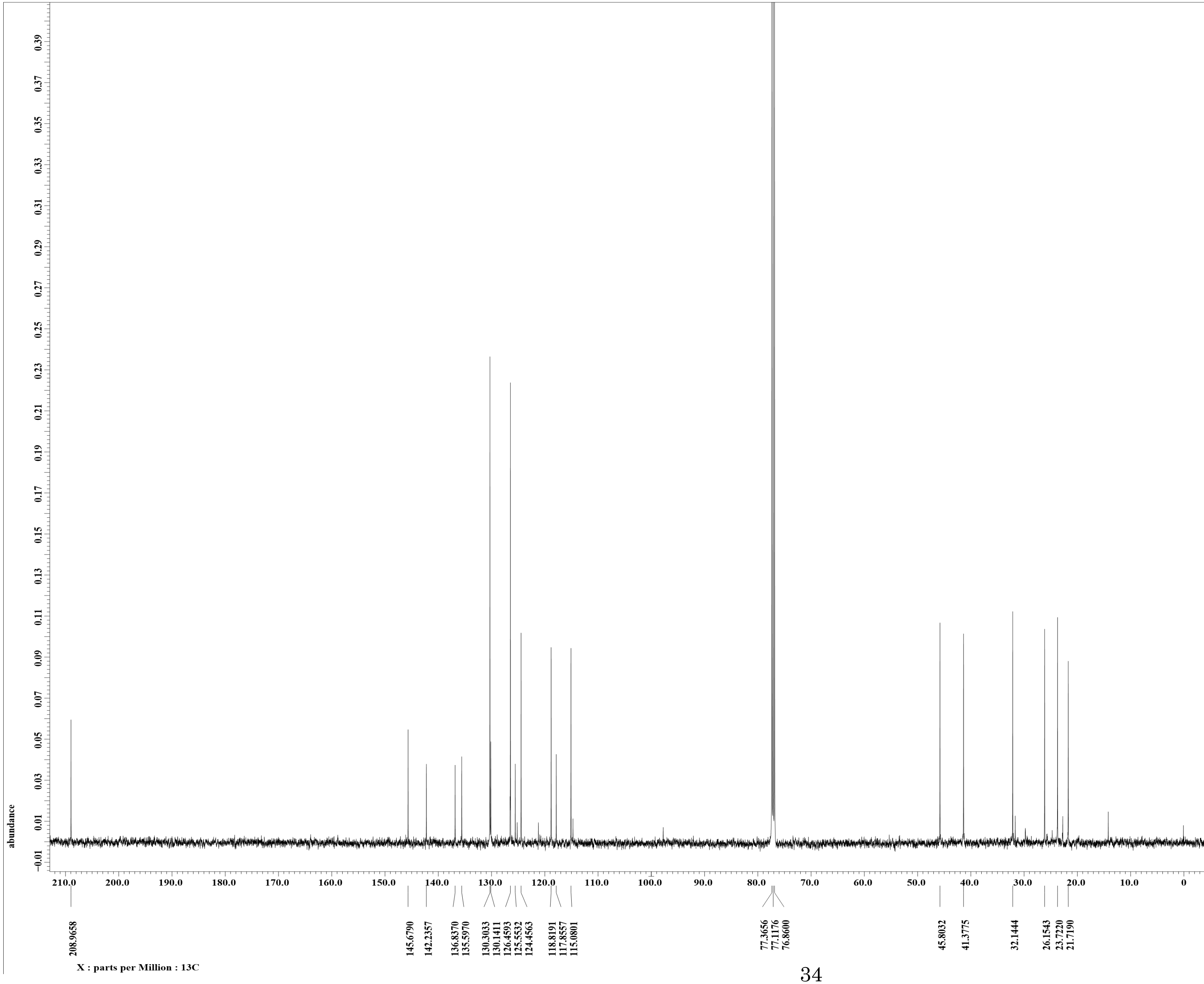

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2020-0323-6Cl-1.jdf
```

Filename	= TA2020-0323-6Cl-5.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#693221
Solvent	= CHLOROFORM-D
Creation_time	= 8-JUN-2000 21:02:08
Revision_time	= 23-MAR-2020 19:19:15
Current_time	= 23-MAR-2020 19:19:43
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	= 23[dC]



3ga




```
---- 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

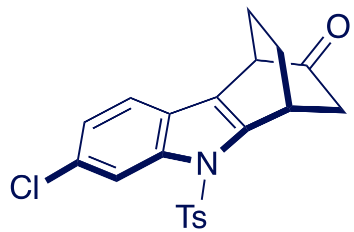
Derived from: TA2020-0325-5.jdf

Filename            = TA2020-0325-7.jdf
Author              = delta
Experiment          = single_pulse_dec
Sample_id           = S#367496
Solvent             = CHLOROFORM-D
Creation_time       = 10-JUN-2000 12:57:47
Revision_time       = 25-MAR-2020 11:12:26
Current_time        = 25-MAR-2020 11:12:58

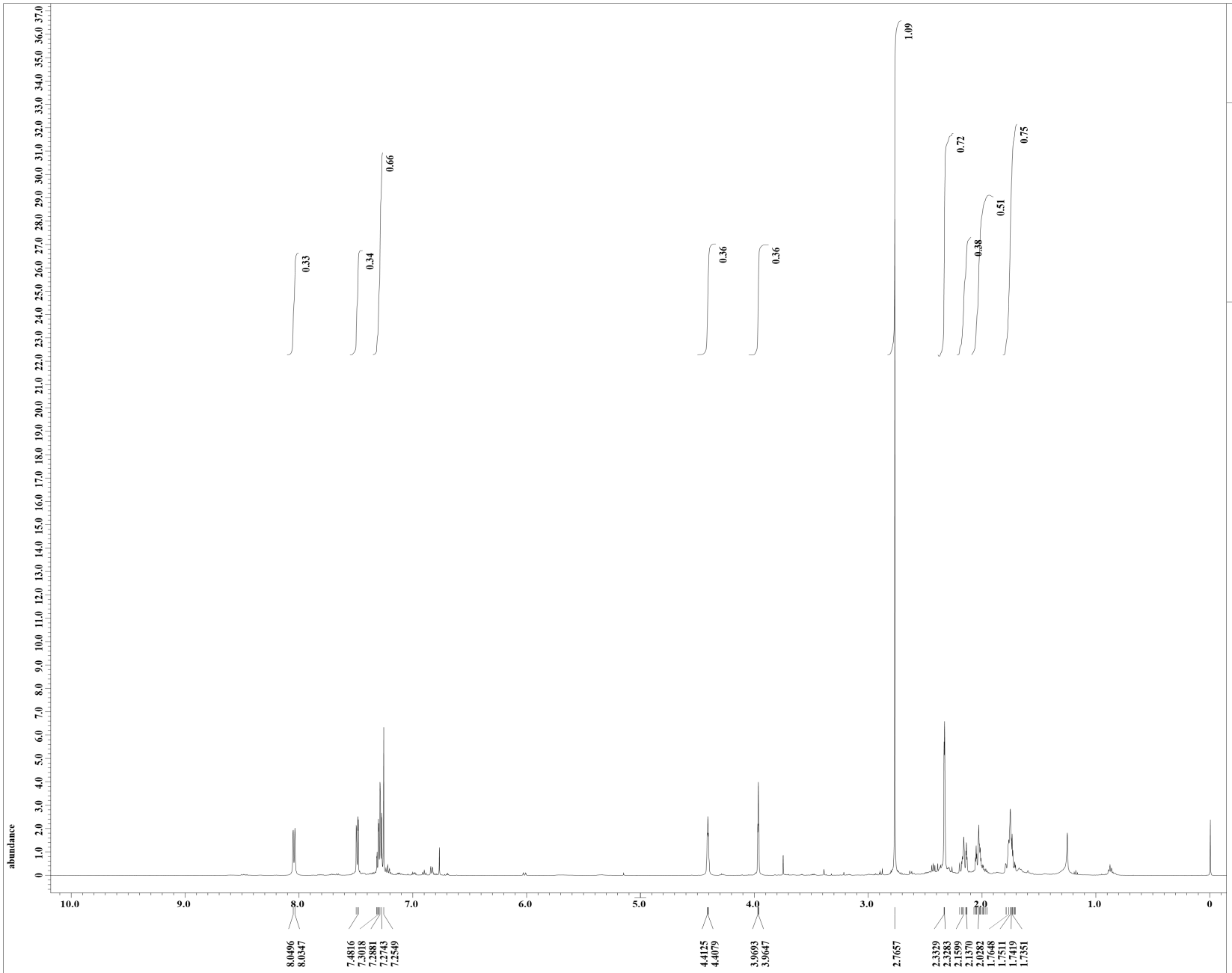
Comment             = single pulse decouple
Data_format         = 1D COMPLEX
Dim_size            = 26214
Dim_title           = 13C
Dim_units           = [ppm]
Dimensions          = X
Site                = ECA500
Spectrometer        = DELTA2_NMR

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               = 1250
Total_scans         = 1250

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            = 24[dC]
```



3ga



```
---- 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

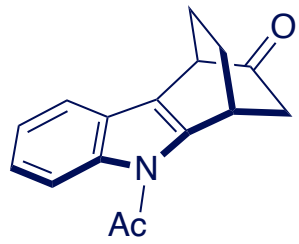
Derived from: TA2020-0330-11.jdf
```

```
Filename          = TA2020-0330-14.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#529365
Solvent           = CHLOROFORM-D
Creation_time     = 15-JUN-2000 16:28:47
Revision_time     = 30-MAR-2020 14:53:53
Current_time      = 30-MAR-2020 14:54:14

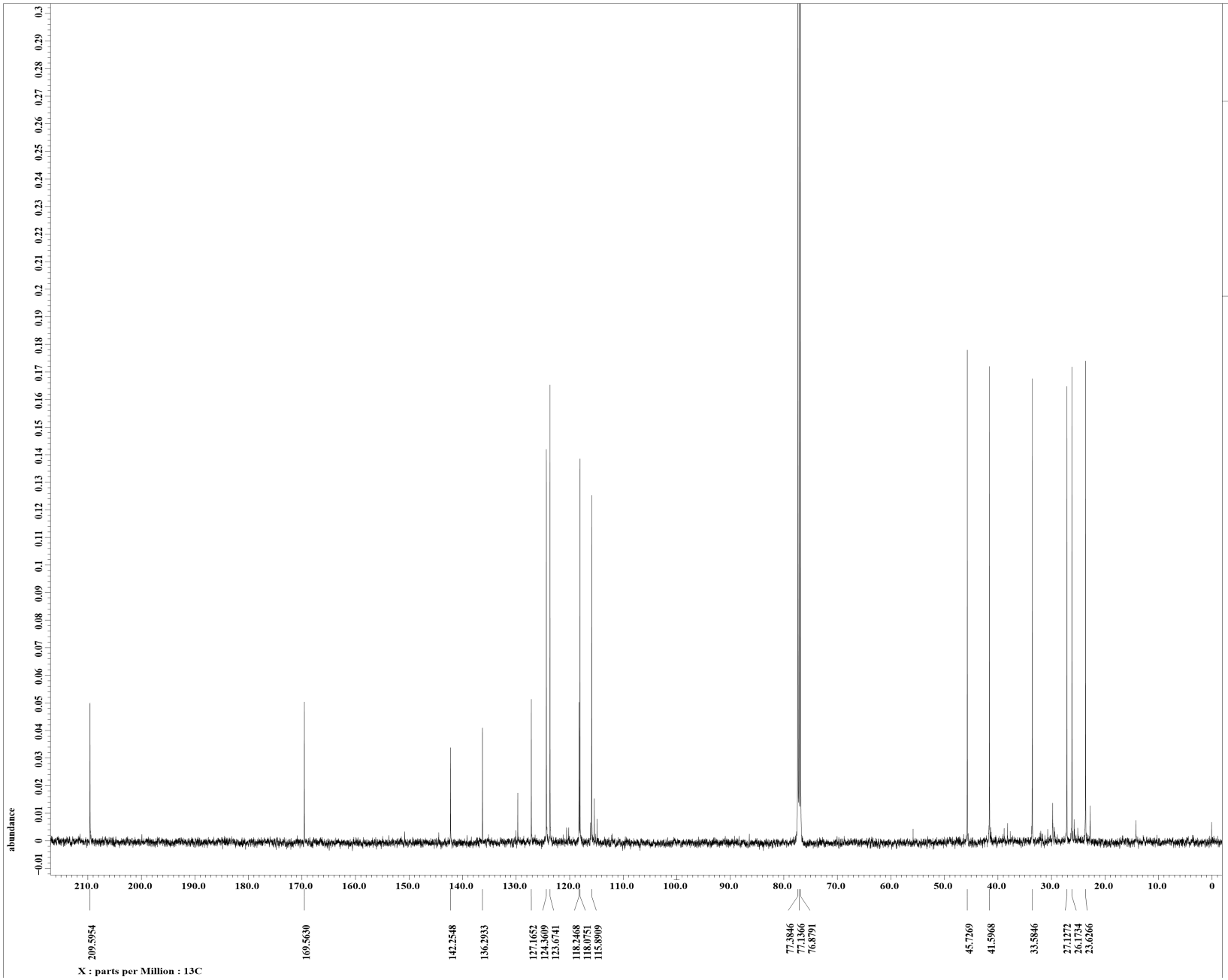
Comment           = Ac-cyclohexene
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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]
```



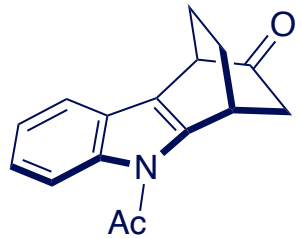
3ia



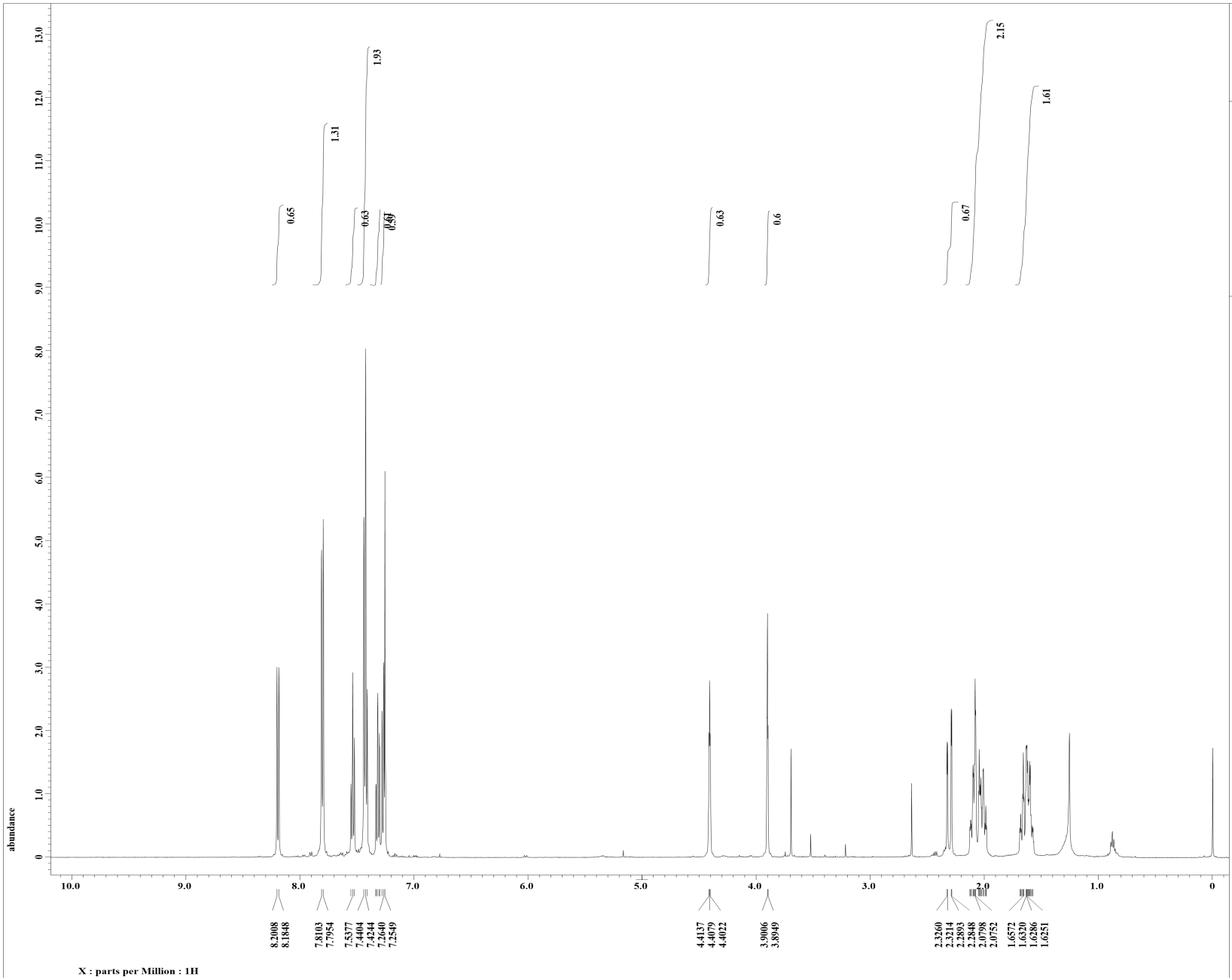
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2020-0330-12.jdf
```

Filename	= TA2020-0330-15.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#530115
Solvent	= CHLOROFORM-D
Creation_time	= 15-JUN-2000 18:18:32
Revision_time	= 30-MAR-2020 16:33:31
Current_time	= 30-MAR-2020 16:35:30
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	= 2307
Total_scans	= 2307
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	= 23.7[dC]



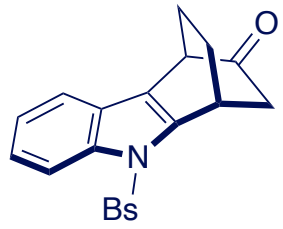
3ia



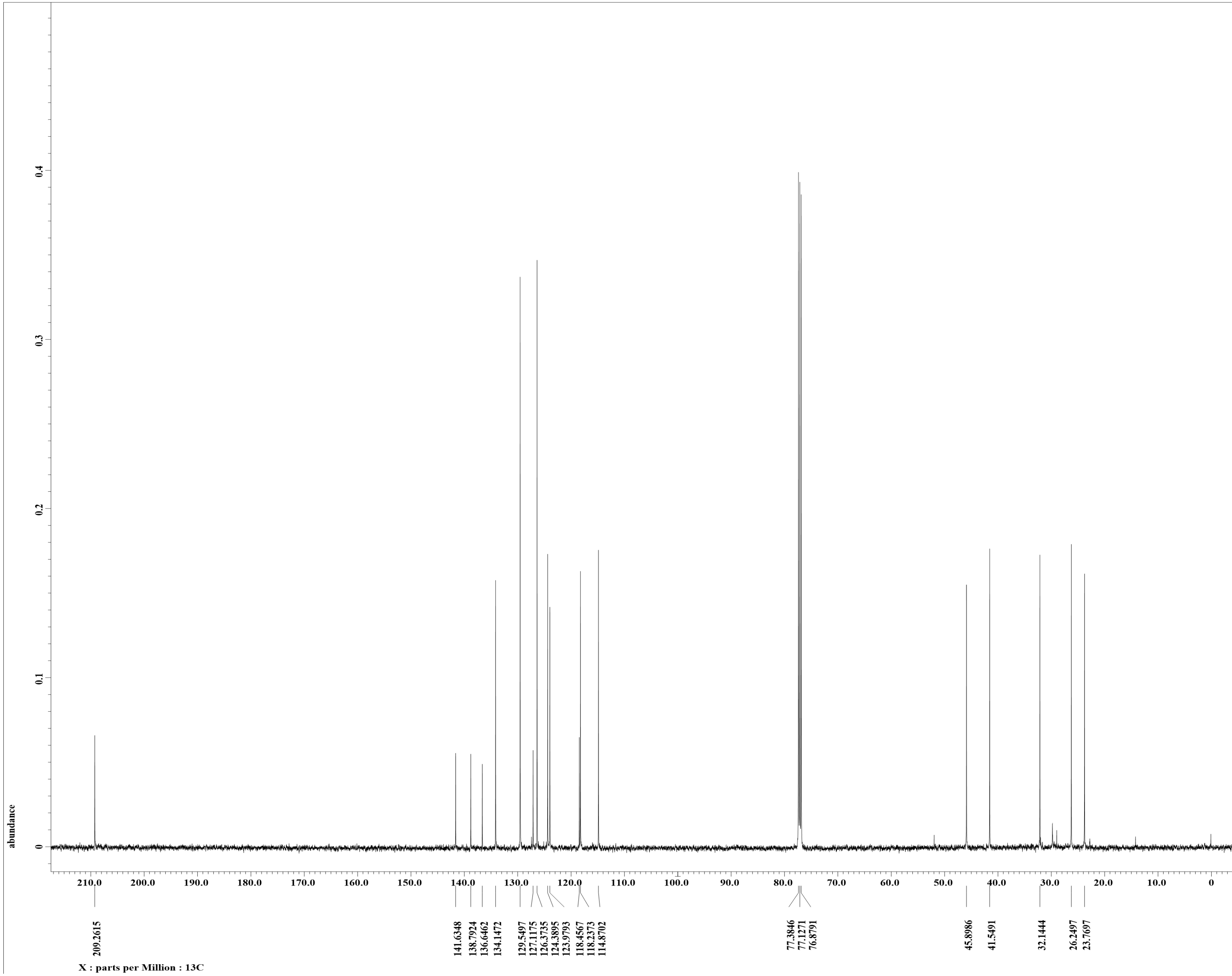
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2020-0416-1.jdf

Filename	= TA2020-0416-9.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#388094
Solvent	= CHLOROFORM-D
Creation_time	= 2-JUL-2000 12:32:45
Revision_time	= 16-APR-2020 11:39:41
Current_time	= 16-APR-2020 11:40:15
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	= 22.9[dC]



3ka




```
---- 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

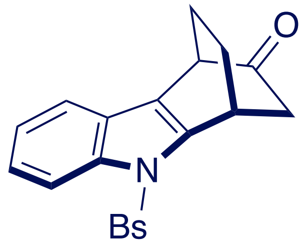
Derived from: TA2020-0416-7.jdf
```

```
Filename          = TA2020-0416-9.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#417885
Solvent           = CHLOROFORM-D
Creation_time     =  2-JUL-2000 15:01:37
Revision_time     = 16-APR-2020 13:17:00
Current_time      = 16-APR-2020 13:17:37

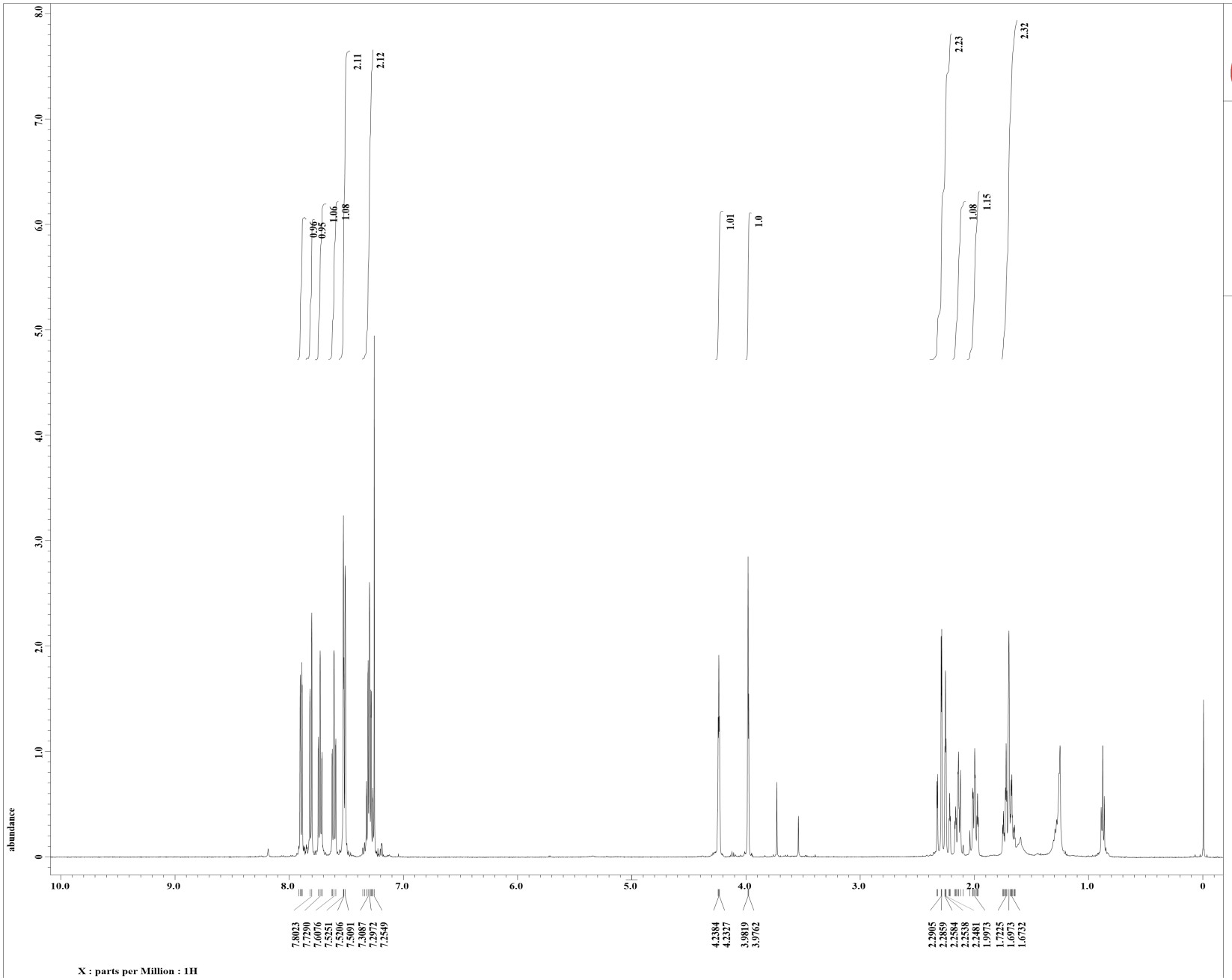
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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           = FALSE
Mod_return        = 1
Scans             = 2110
Total_scans       = 2110

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]
```



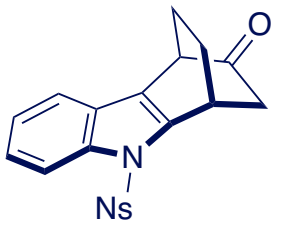
3ka



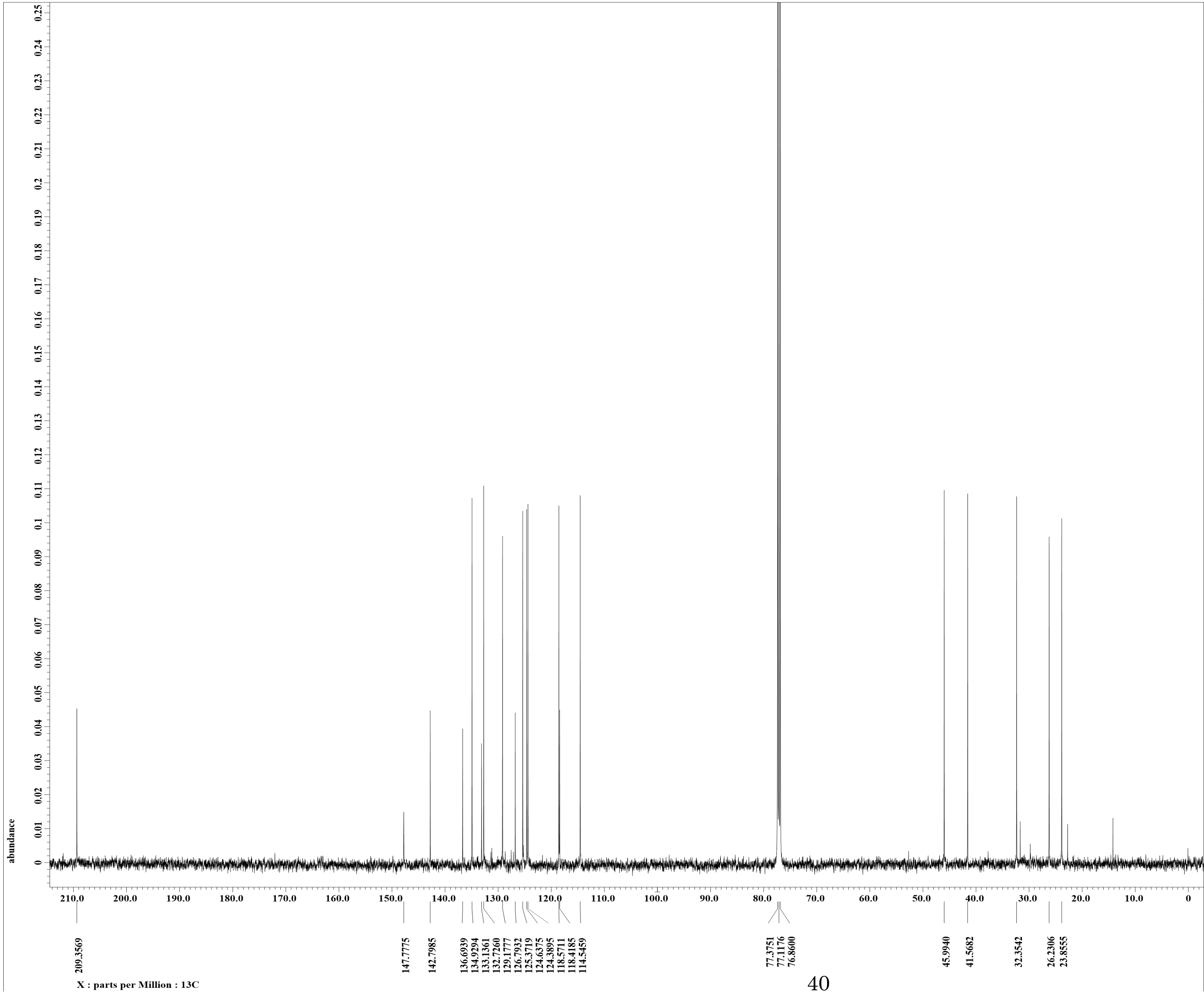

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2020-0328-1.jdf
```

Filename	= TA2020-0328-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#563525
Solvent	= CHLOROFORM-D
Creation_time	= 13-JUN-2000 17:25:47
Revision_time	= 28-MAR-2020 15:45:34
Current_time	= 28-MAR-2020 15:46:36
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	= 22.9[dC]



3la




```
---- 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

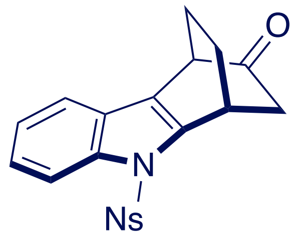
Derived from: TA2020-0328-2.jdf
```

```
Filename          = TA2020-0328-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#564971
Solvent           = CHLOROFORM-D
Creation_time     = 13-JUN-2000 18:59:46
Revision_time     = 28-MAR-2020 17:15:47
Current_time      = 28-MAR-2020 17:16:48

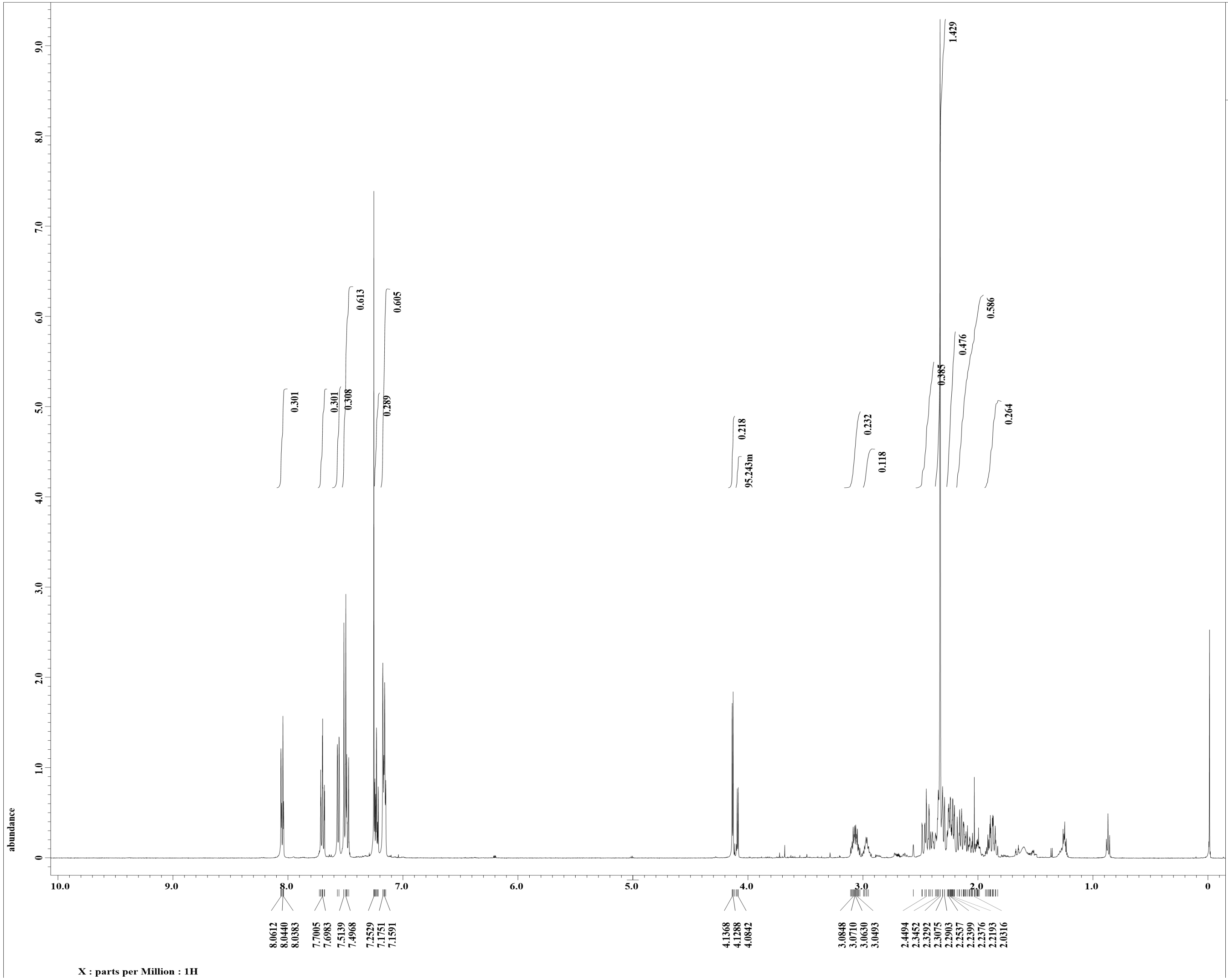
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

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             = 1946
Total_scans       = 1946

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          = 23.8[dC]
```



3la

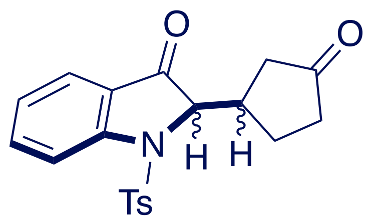



```
Filename           = TA200318-12.jdf
Author             = delta
Experiment         = single_pulse.ex2
Sample_id          = S#681304
Solvent            = CHLOROFORM-D
Creation_time      = 18-MAR-2020 18:03:50
Revision_time      = 18-MAR-2020 19:06:25
Current_time       = 18-MAR-2020 19:07:05

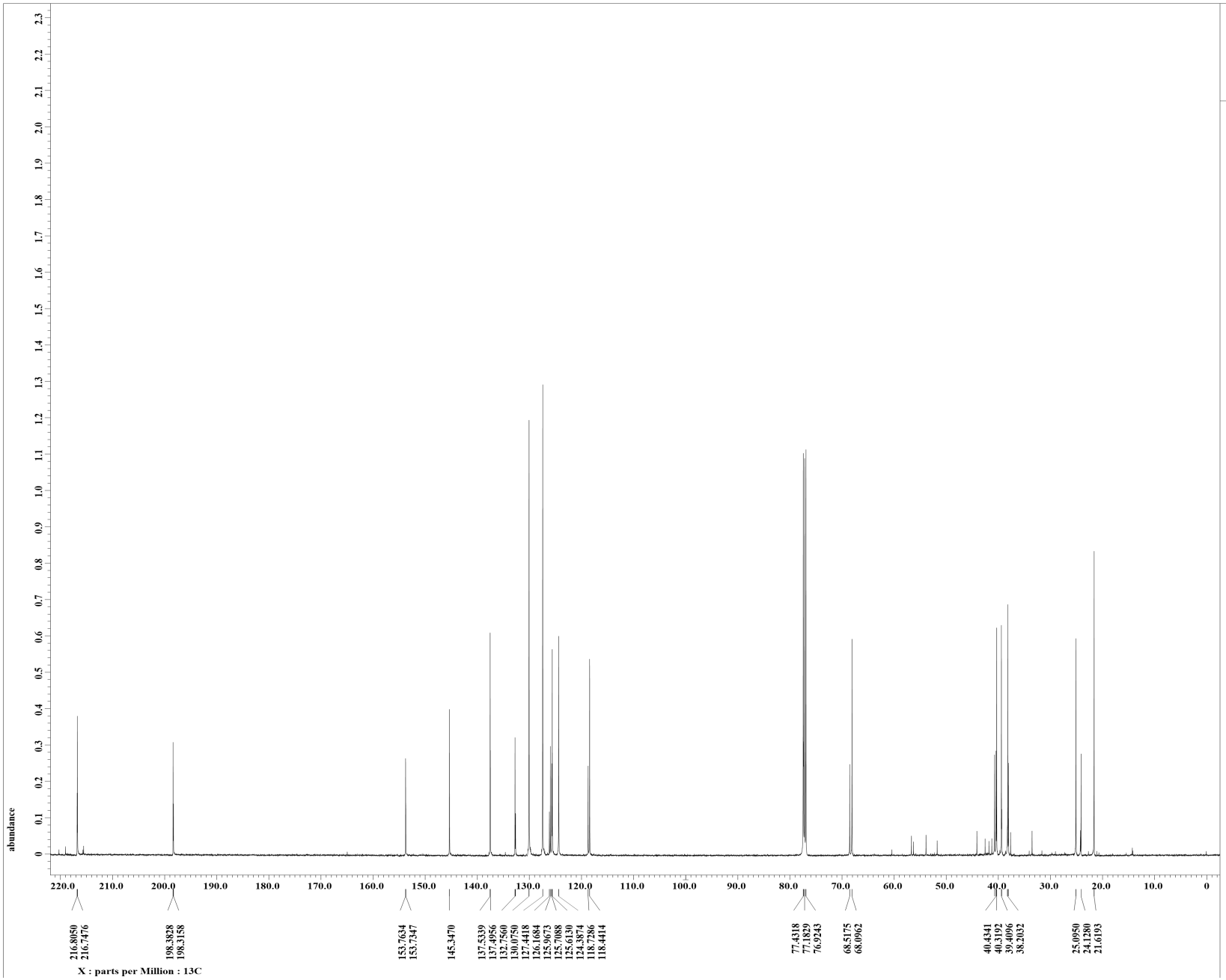
Content            = single_pulse
Data_format        = 1D COMPLEX
Dim_size           = 13107
Dim_title          = 1H
Dim_units          = [ppm]
Dimensions         = X
Site               = ECA 500
Spectrometer       = DELTA2_NMR

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           = 23.7[dC]
```



3ab

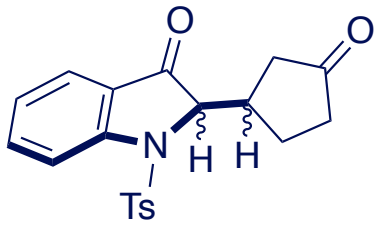


Filename = TA200318-16.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#69383
Solvent = CHLOROFORM-D
Creation_time = 19-MAR-2020 07:34:03
Revision_time = 19-MAR-2020 08:28:18
Current_time = 19-MAR-2020 08:29:17

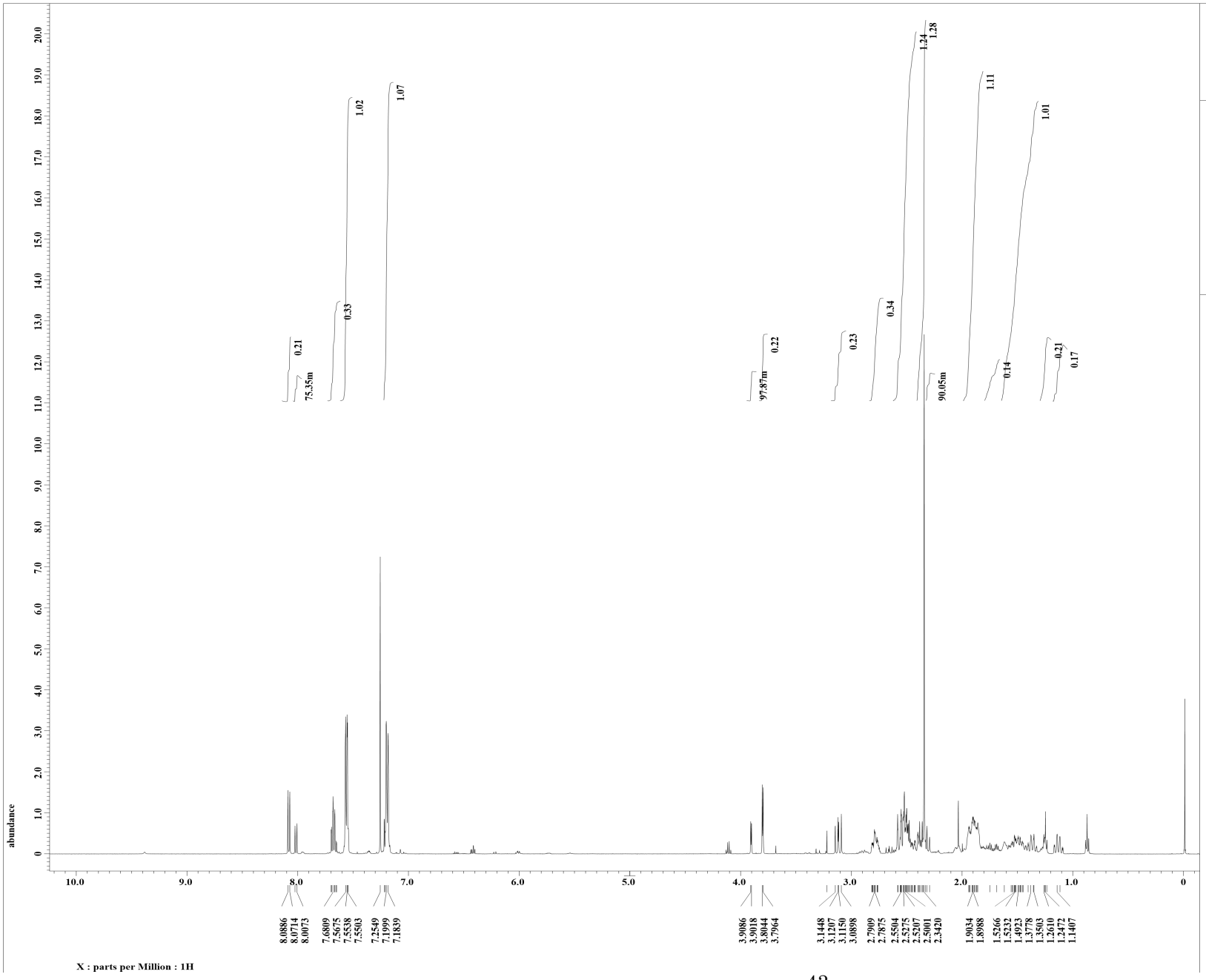
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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 = 16705
Total_scans = 16705

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 = 24.3[dC]



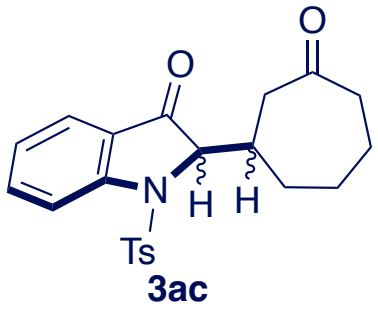
3ab



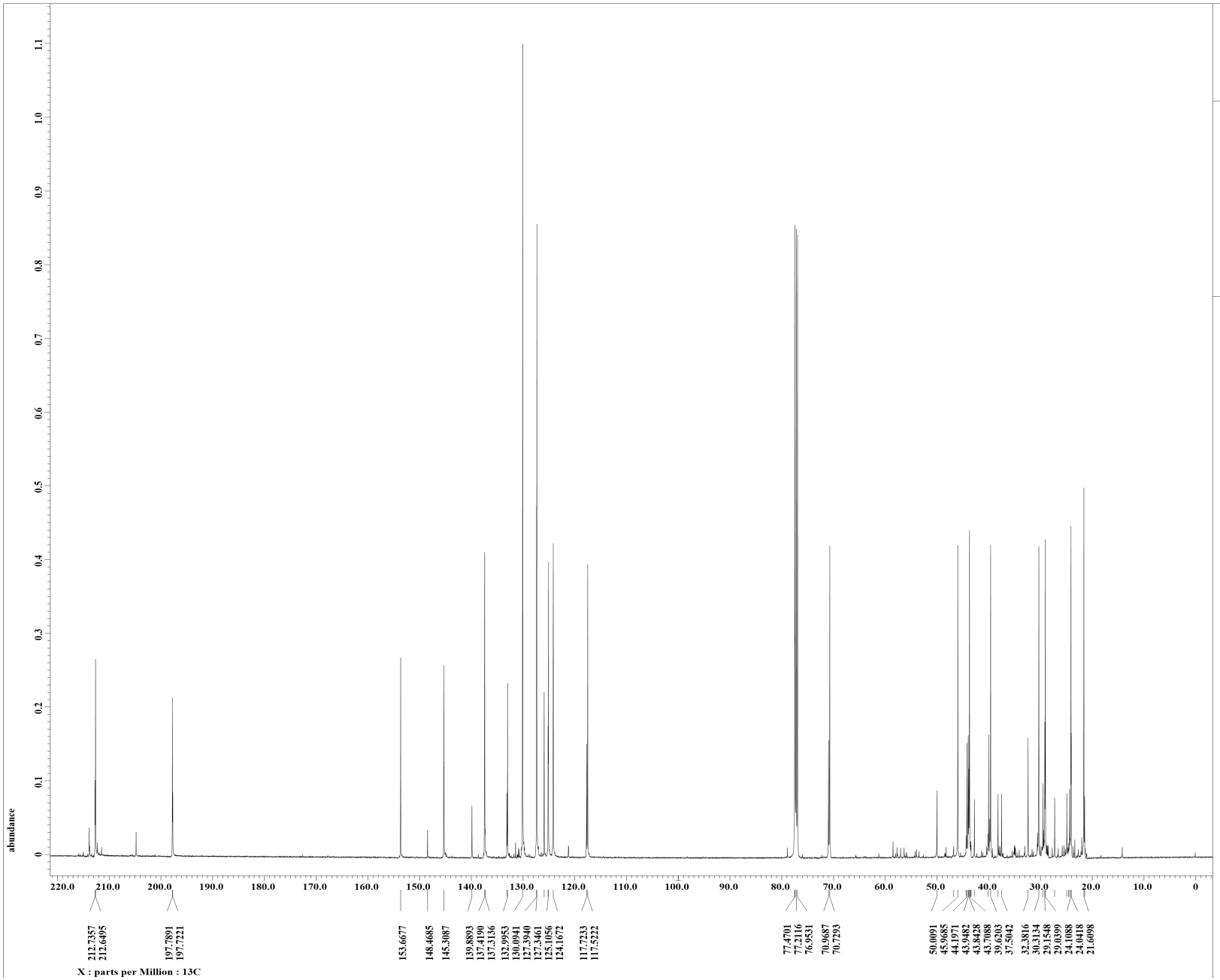

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA2020-0319-1.jdf
```

Filename	= TA2020-0319-5.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#462109
Solvent	= CHLOROFORM-D
Creation_time	= 4-JUN-2000 14:37:04
Revision_time	= 19-MAR-2020 13:00:59
Current_time	= 19-MAR-2020 13:01:55
Comment	= cycloheptenone
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	= 22.7[dC]



3ac




```
---- 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

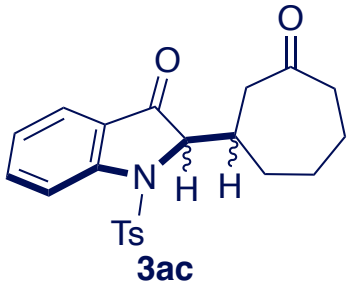
Derived from: TA200320-2-4.jdf
```

```
Filename          = TA200320-2-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#567161
Solvent           = CHLOROFORM-D
Creation_time     = 23-MAR-2020 07:33:39
Revision_time     = 26-APR-2020 11:49:23
Current_time      = 26-APR-2020 11:50:30

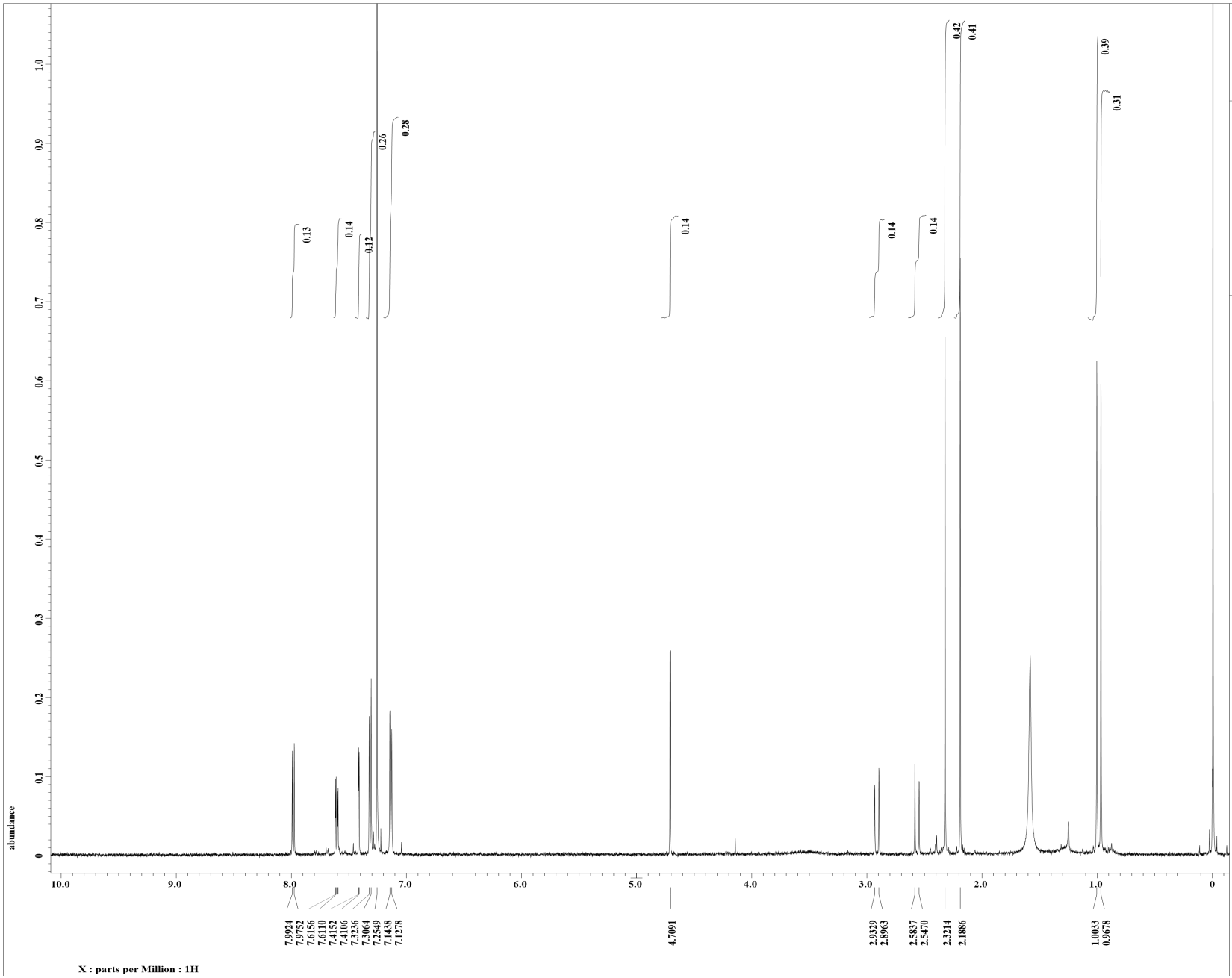
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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             = 82030
Total_scans       = 82030

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        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 2.8388608[s]
Temp_get          = 24[dC]
```

3ac



---- 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

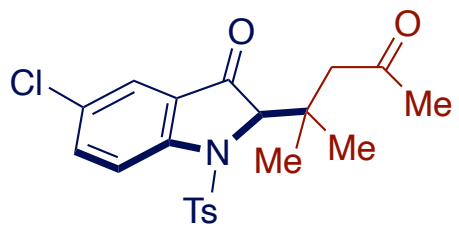
Derived from: 5Cl-acetone-1H-1.jdf

Filename = 5Cl-acetone-1H-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#633038
Solvent = CHLOROFORM-D
Creation_time = 5-MAY-2000 19:22:58
Revision_time = 18-FEB-2020 17:40:51
Current_time = 18-FEB-2020 17:41:14

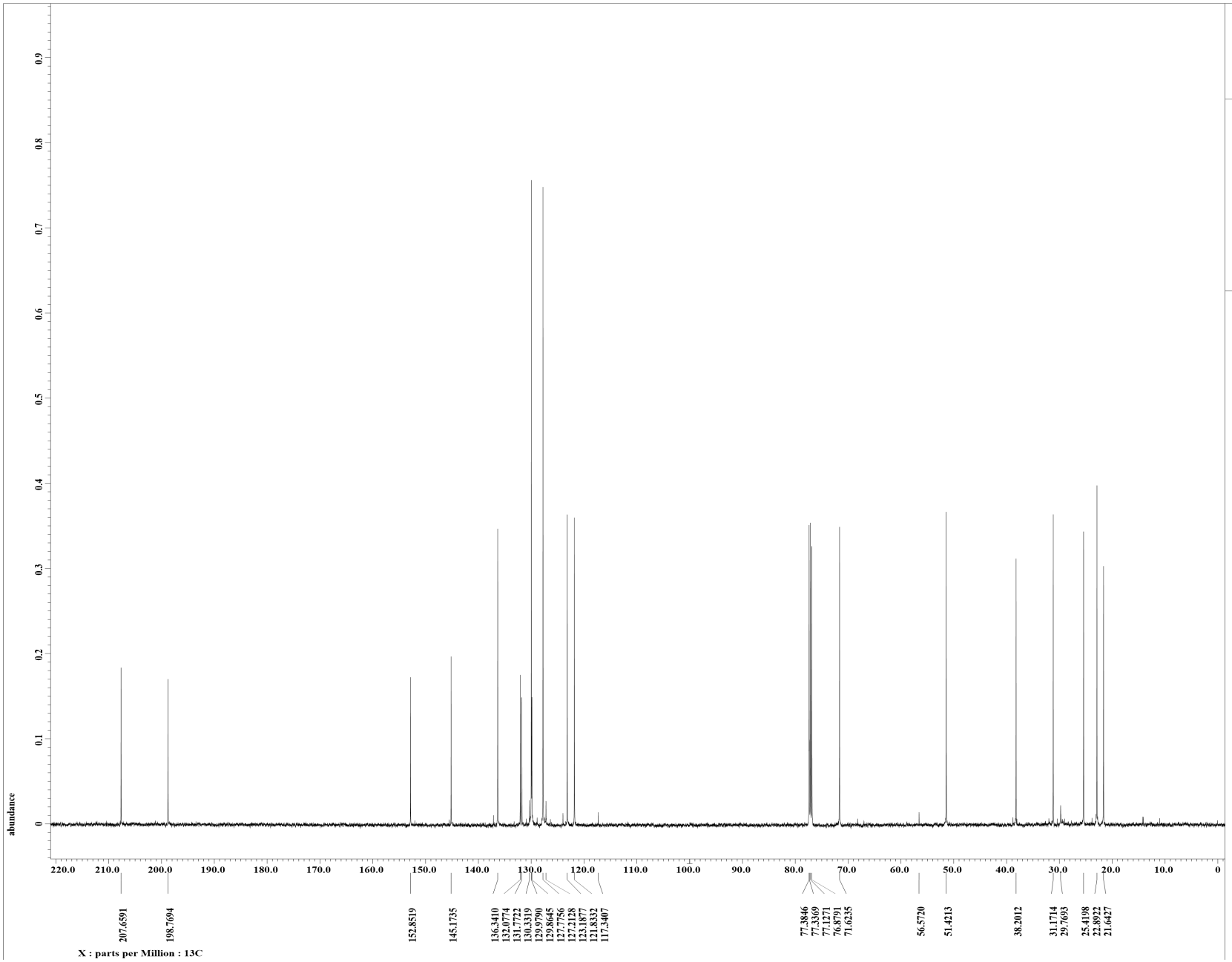
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA500
Spectrometer = DELTA2_NMR

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 = 23[dC]



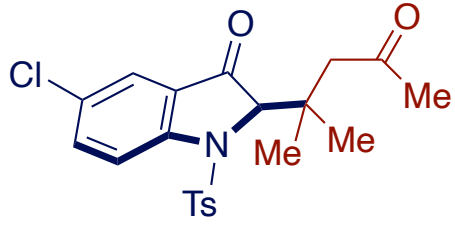
3bf



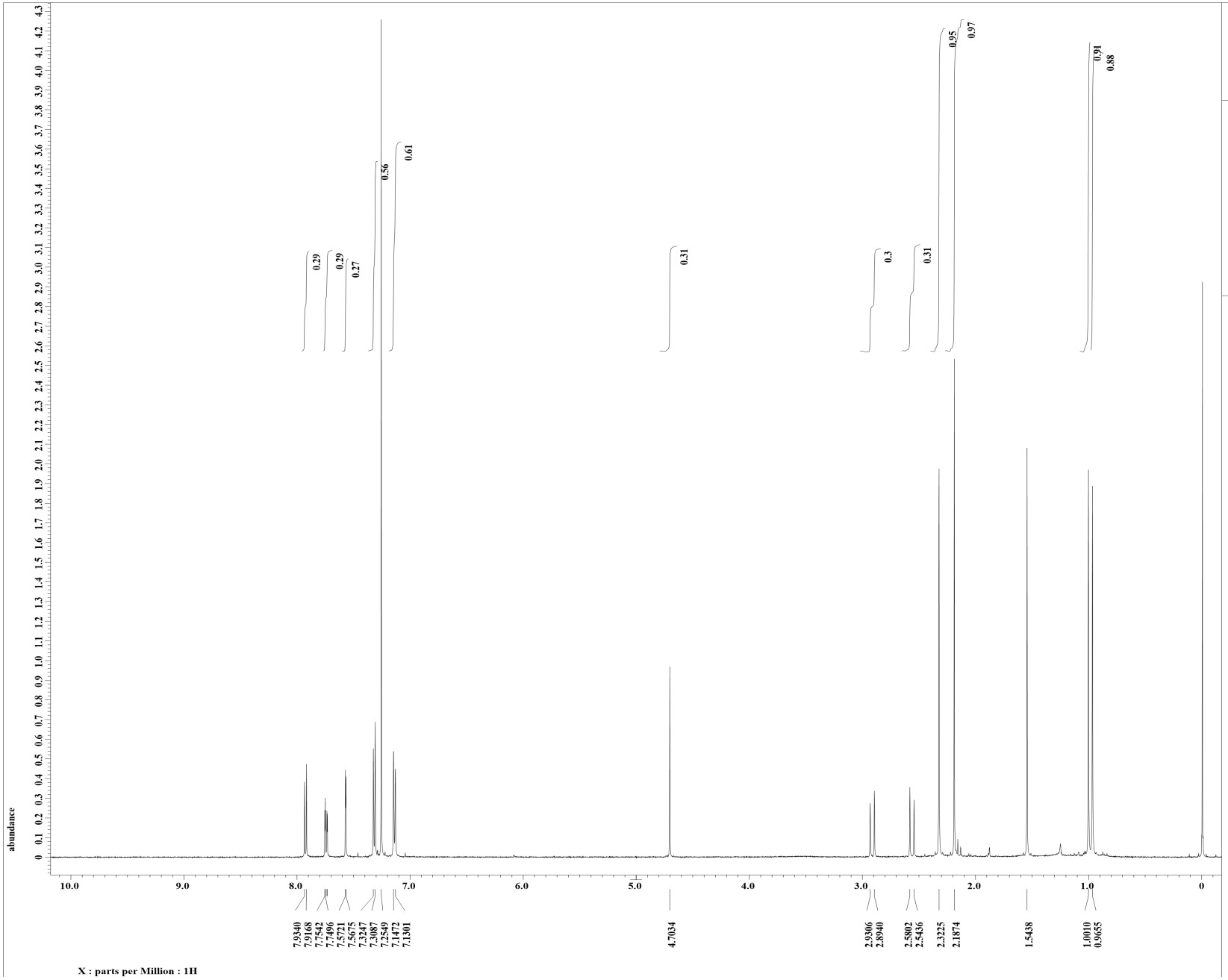

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 5Cl-acetone-13C-1.jdf
```

Filename	= 5Cl-acetone-13C-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#636019
Solvent	= CHLOROFORM-D
Creation_time	= 5-MAY-2000 20:55:10
Revision_time	= 18-FEB-2020 19:08:26
Current_time	= 18-FEB-2020 19:09:02
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	= 1857
Total_scans	= 1857
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	= 23.6[dC]



3bf




```
---- 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

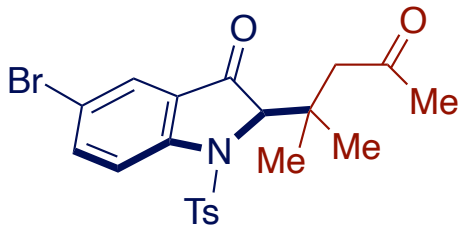
Derived from: 5Br-acetone-1H-4.jdf
```

```
Filename            = 5Br-acetone-1H-7.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_id           = S#392432
Solvent             = CHLOROFORM-D
Creation_time       =  6-MAY-2000 12:41:56
Revision_time       = 19-FEB-2020 10:58:41
Current_time        = 19-FEB-2020 10:59:38

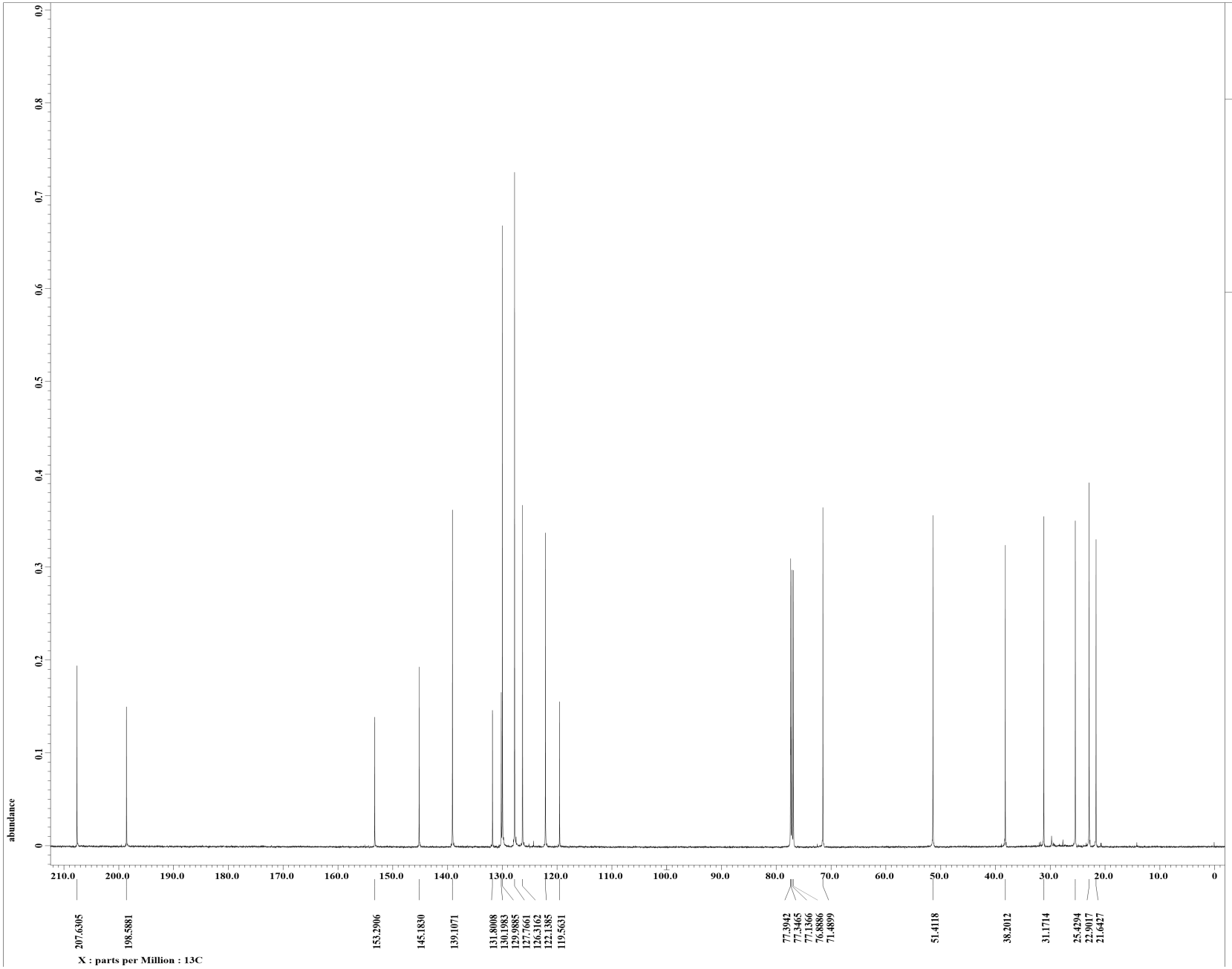
Comment             = 5Br-acetone
Data_format         = 1D COMPLEX
Dim_size            = 13107
Dim_title           = 1H
Dim_units           = [ppm]
Dimensions          = X
Site                = ECA500
Spectrometer        = DELTA2_NMR

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            = 23[dC]
```



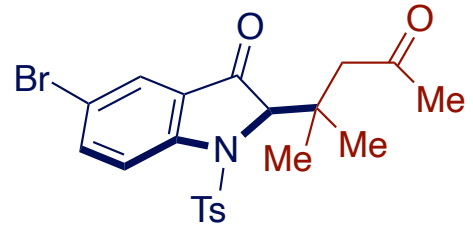
3cf



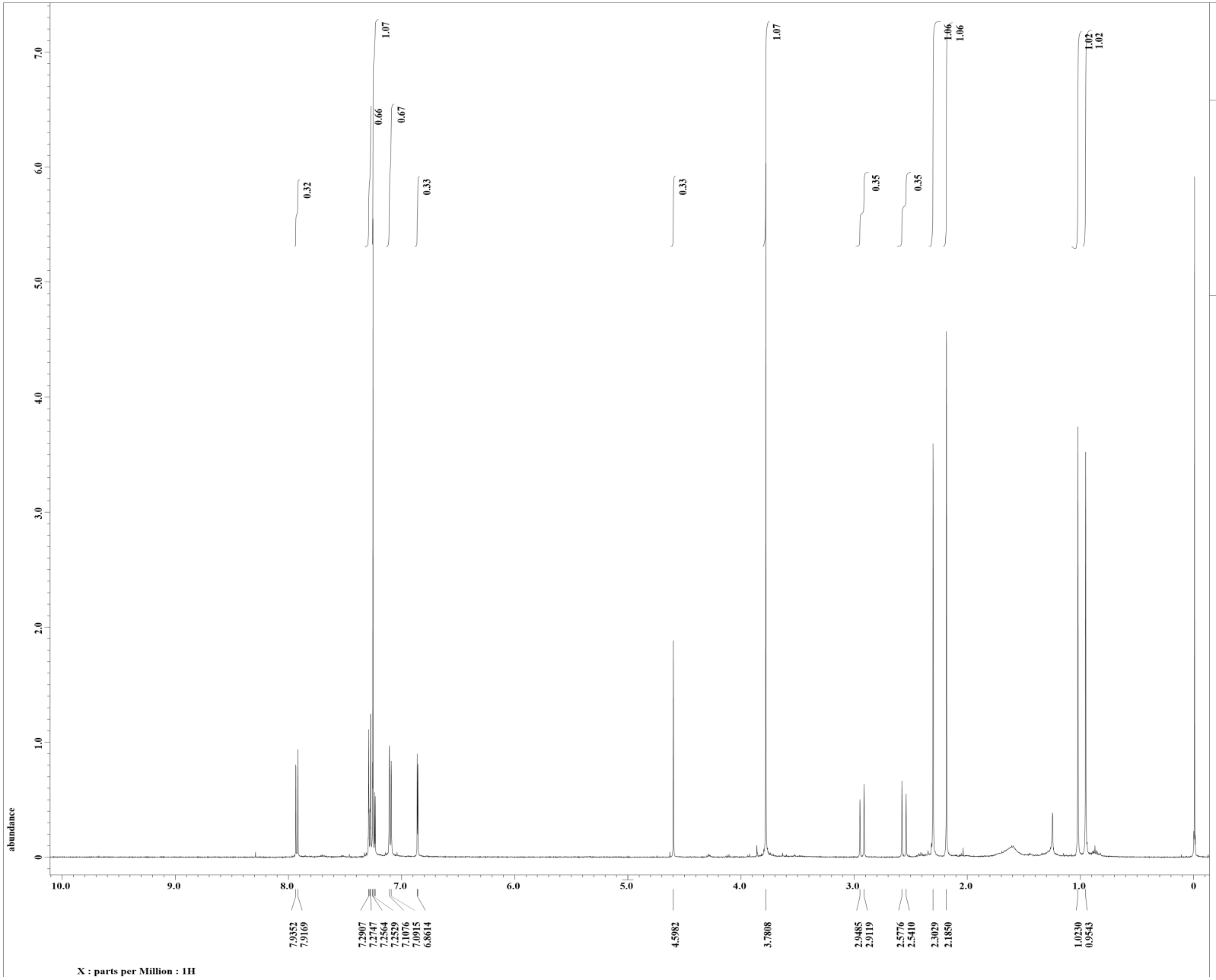

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 5Br-acetone(pure)-13C-1.jd
```

Filename	= 5Br-acetone(pure)-13C
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#705778
Solvent	= CHLOROFORM-D
Creation_time	= 7-MAY-2000 08:59:09
Revision_time	= 20-FEB-2020 07:14:09
Current_time	= 20-FEB-2020 07:14:49
Comment	= 5Br-acetone-13C
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	= 14726
Total_scans	= 14726
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	= 24.6[dC]



3cf



```
---- 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

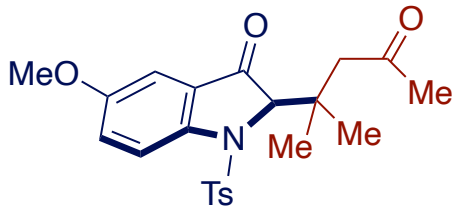
Derived from: TA191125-4-1.jdf
```

```
Filename          = TA191125-4-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#485579
Solvent           = CHLOROFORM-D
Creation_time     = 25-NOV-2019 12:45:24
Revision_time     =  7-MAY-2020 15:41:02
Current_time      =  7-MAY-2020 15:41:31

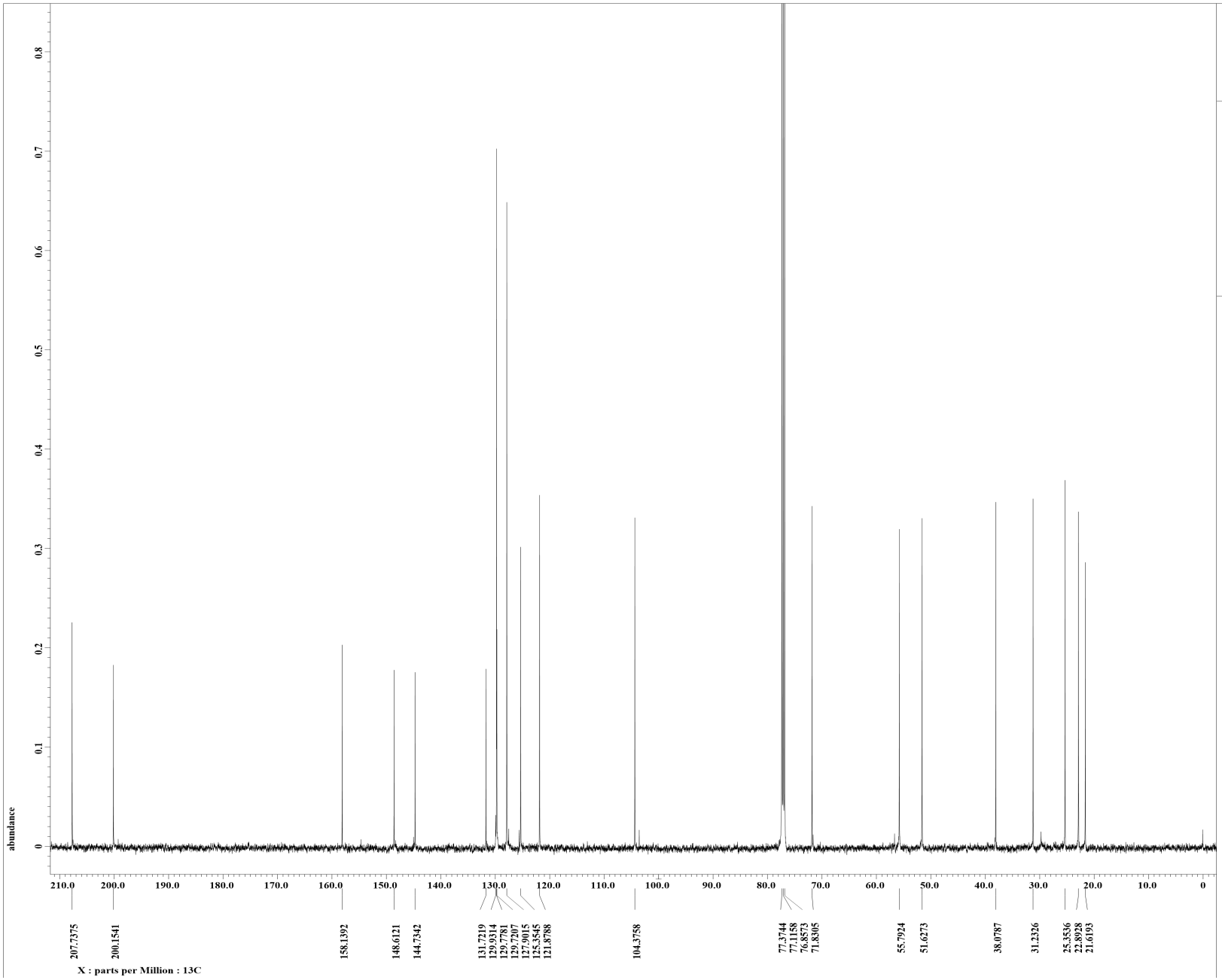
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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          = 23.7[dC]
```



3df




```
---- 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: TA191125_copy-1.jdf
```

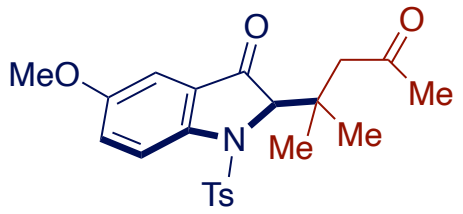


```
Filename          = TA191125_copy-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#621540
Solvent           = CHLOROFORM-D
Creation_time     = 25-NOV-2019 19:05:34
Revision_time     =  7-MAY-2020 15:43:58
Current_time      =  7-MAY-2020 15:44:37

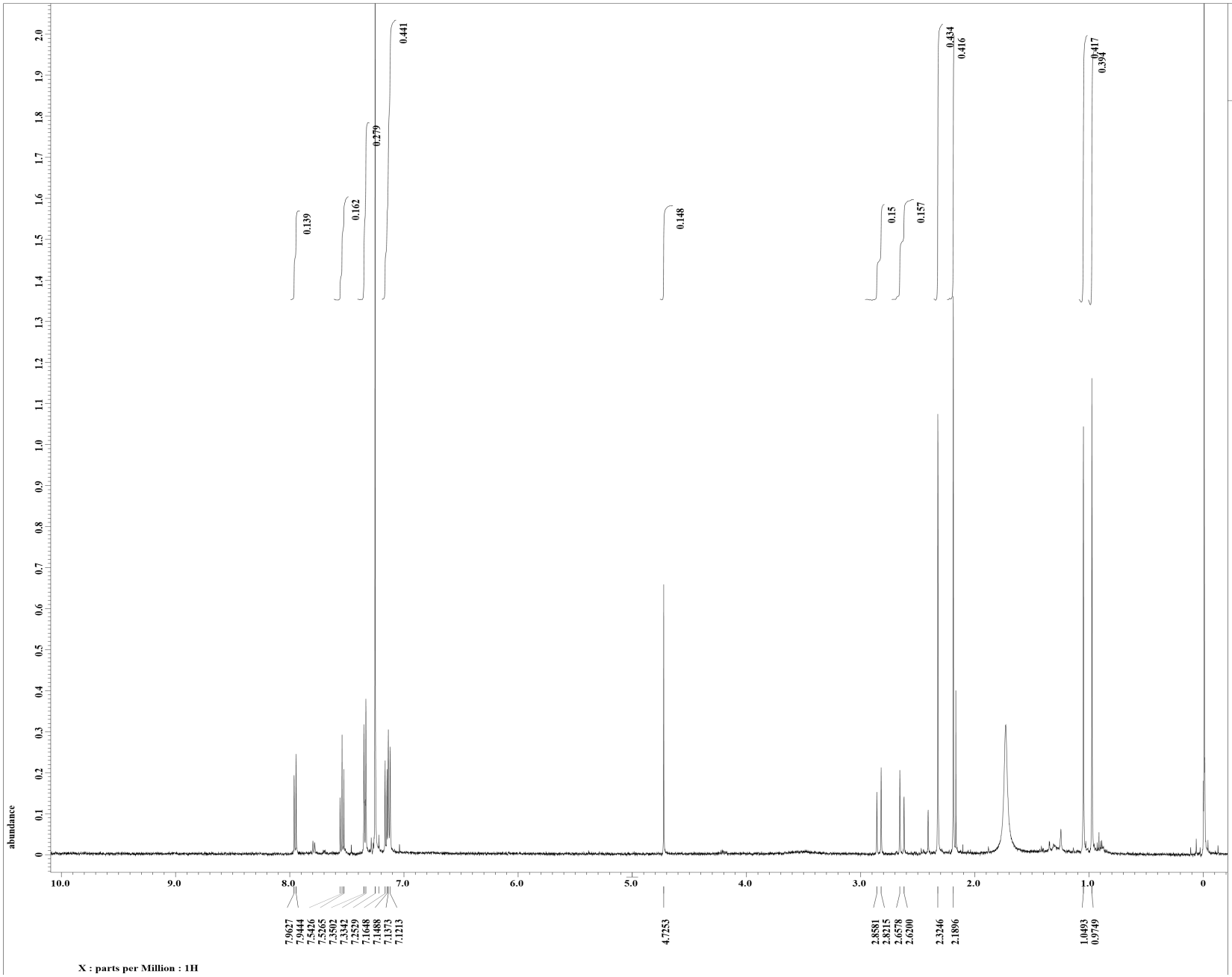
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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           = TRUE
Incomplete_copy   = TRUE
Mod_return        = 1
Scans             = 3253
Total_scans       = 3253

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          = 24.3[dC]
```

3df

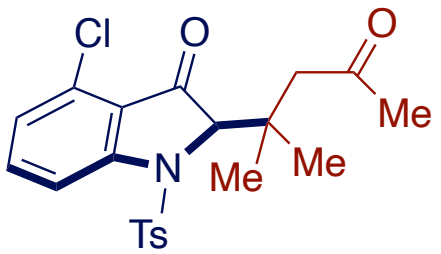


Filename = 4-Cl-acetone-1H-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#645124
Solvent = CHLOROFORM-D
Creation_time = 15-FEB-2020 16:59:05
Revision_time = 15-FEB-2020 18:01:13
Current_time = 15-FEB-2020 18:01:33

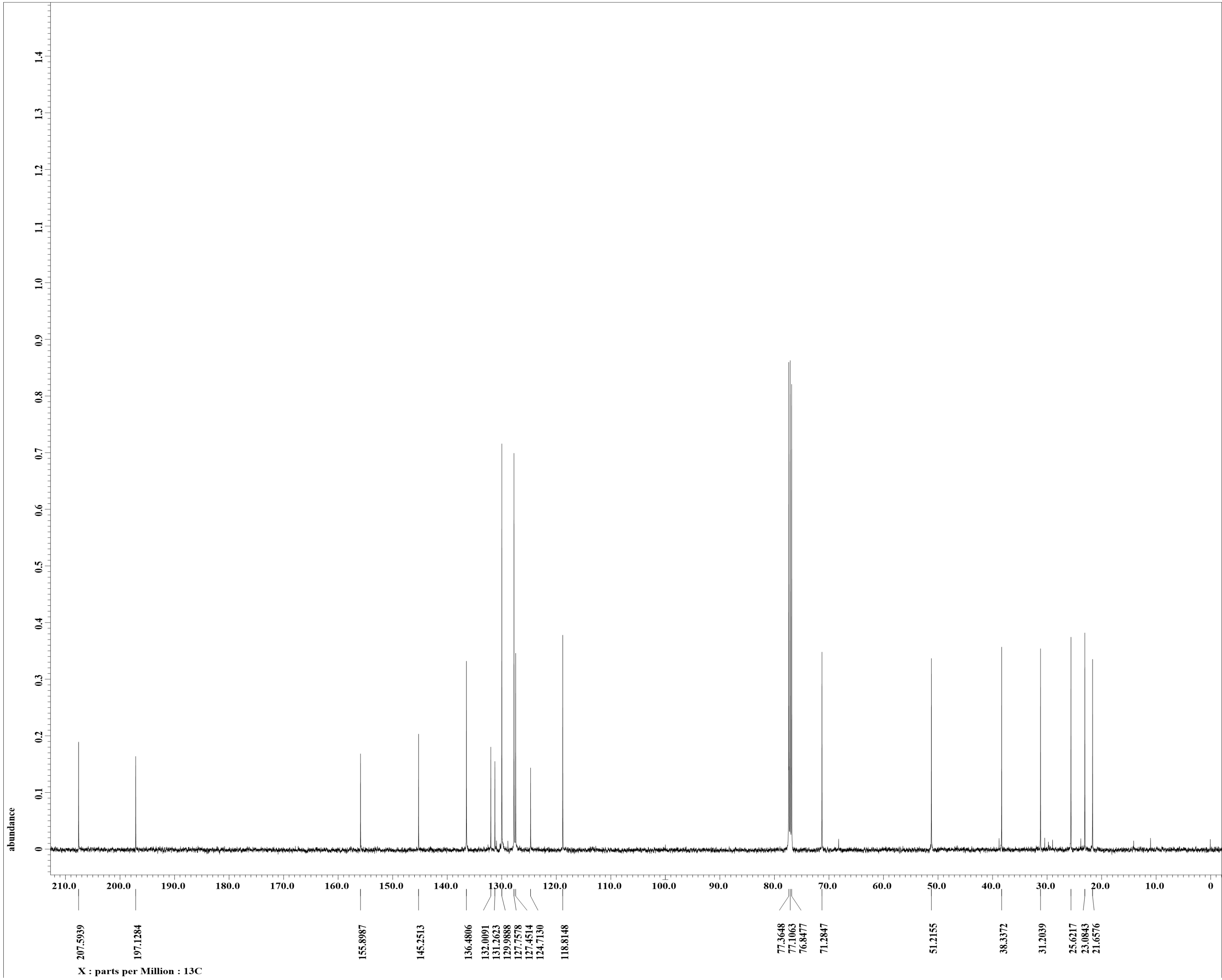
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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 = 23.7[dC]



3ff

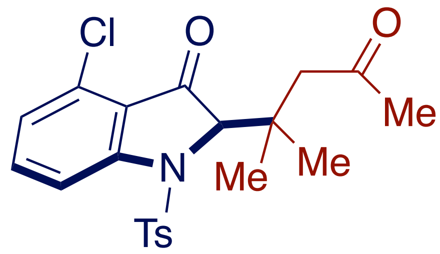



```
Filename          = 4Cl-acetone-13C-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#648306
Solvent           = CHLOROFORM-D
Creation_time     = 15-FEB-2020 19:08:05
Revision_time     = 15-FEB-2020 20:06:10
Current_time      = 15-FEB-2020 20:06:43

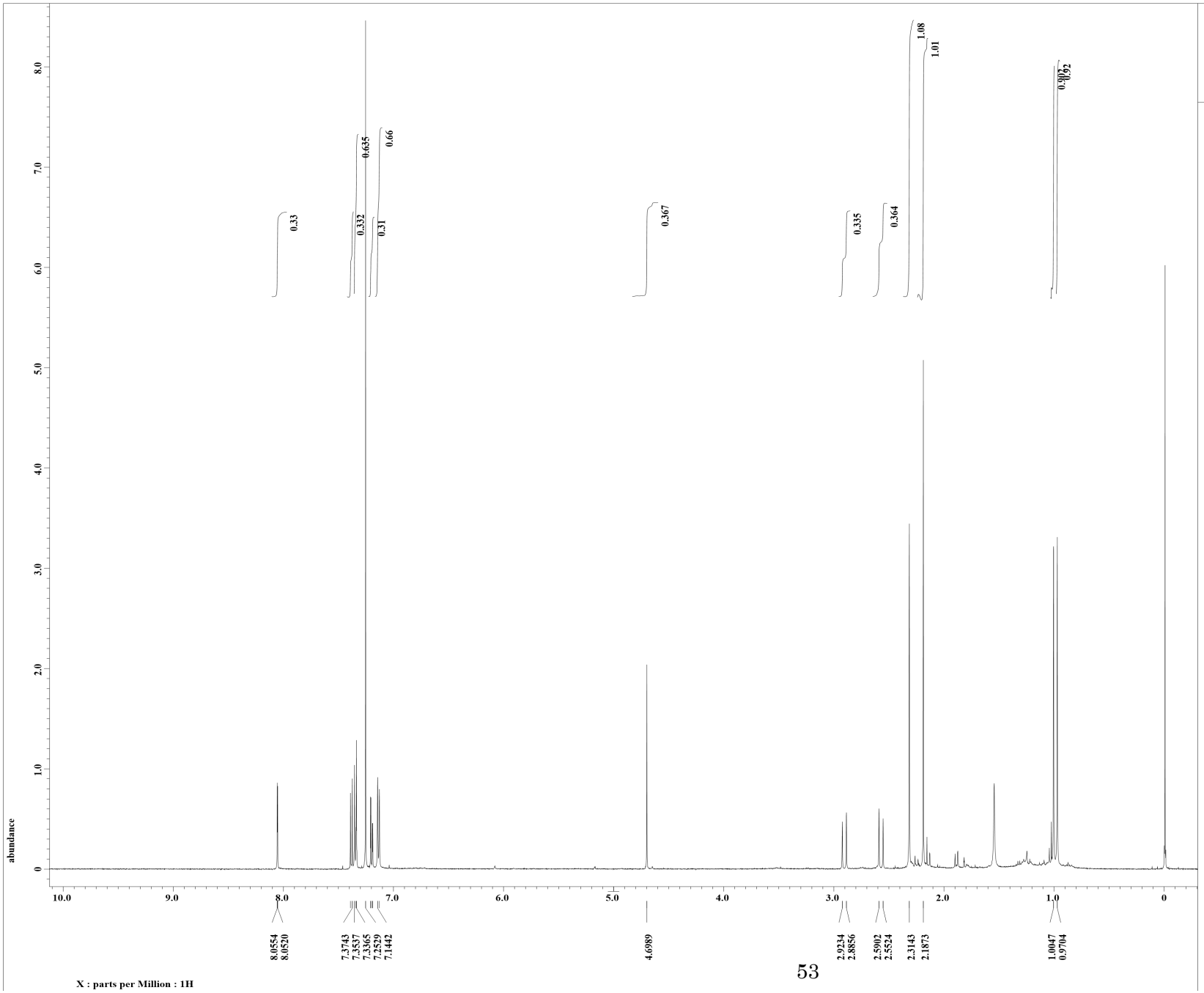
Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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             = 2624
Total_scans       = 2624

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]
```



3ff

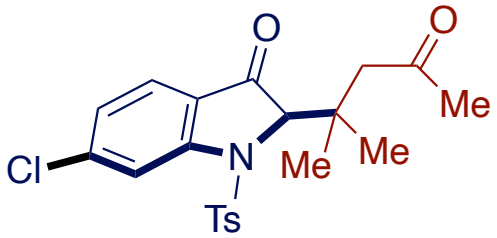


Filename = 6-Cl-acetone-1H-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#664518
Solvent = CHLOROFORM-D
Creation_time = 21-FEB-2020 17:30:24
Revision_time = 21-FEB-2020 18:32:59
Current_time = 21-FEB-2020 18:33:17

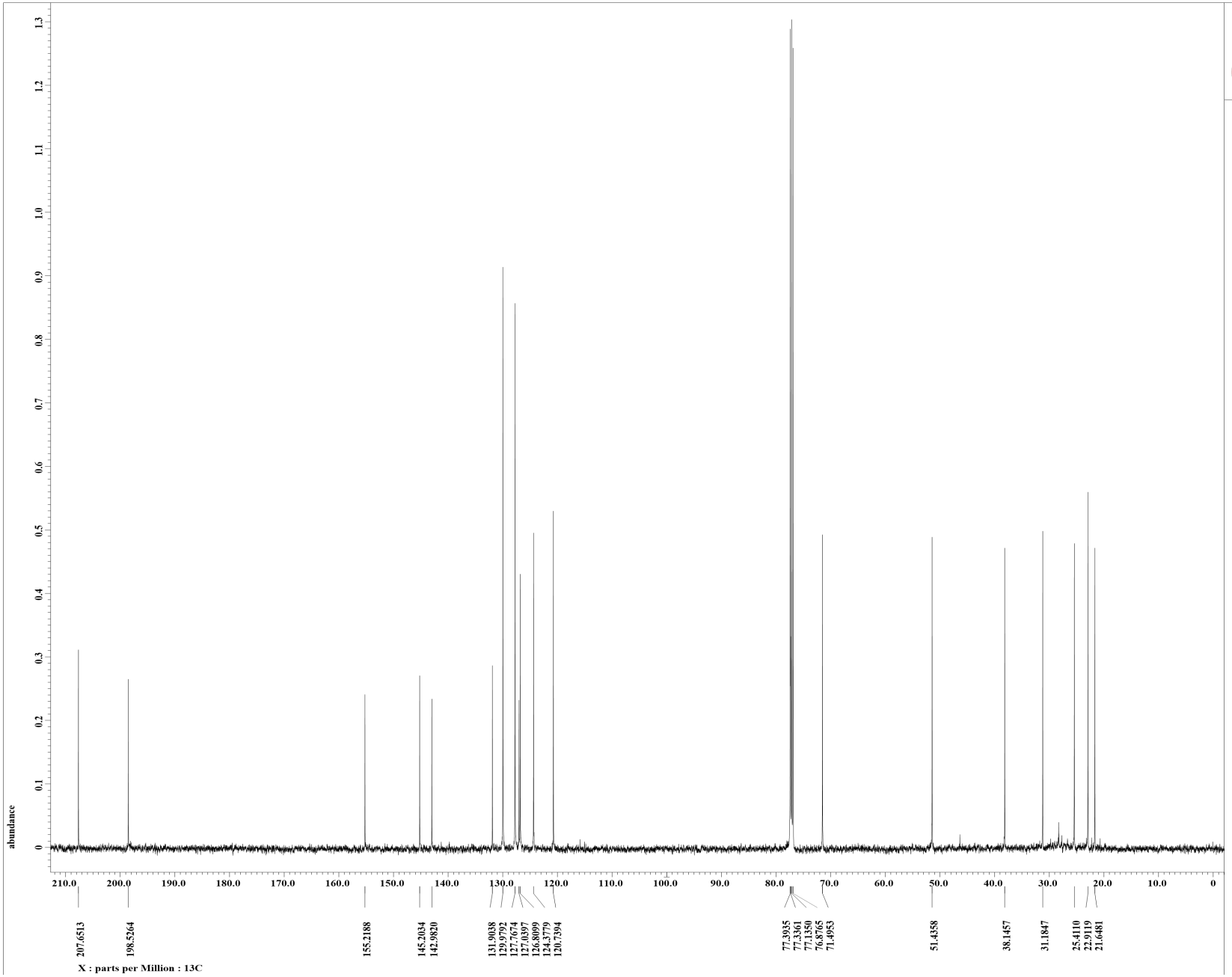
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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 = 23.6[dC]



3gf

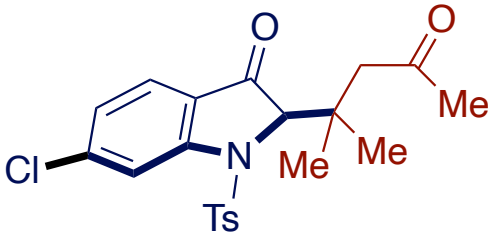



```
Filename          = 6-Cl-acetone-13C-2.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#668031
Solvent           = CHLOROFORM-D
Creation_time     = 21-FEB-2020 18:40:10
Revision_time     = 21-FEB-2020 19:39:03
Current_time      = 21-FEB-2020 19:39:48

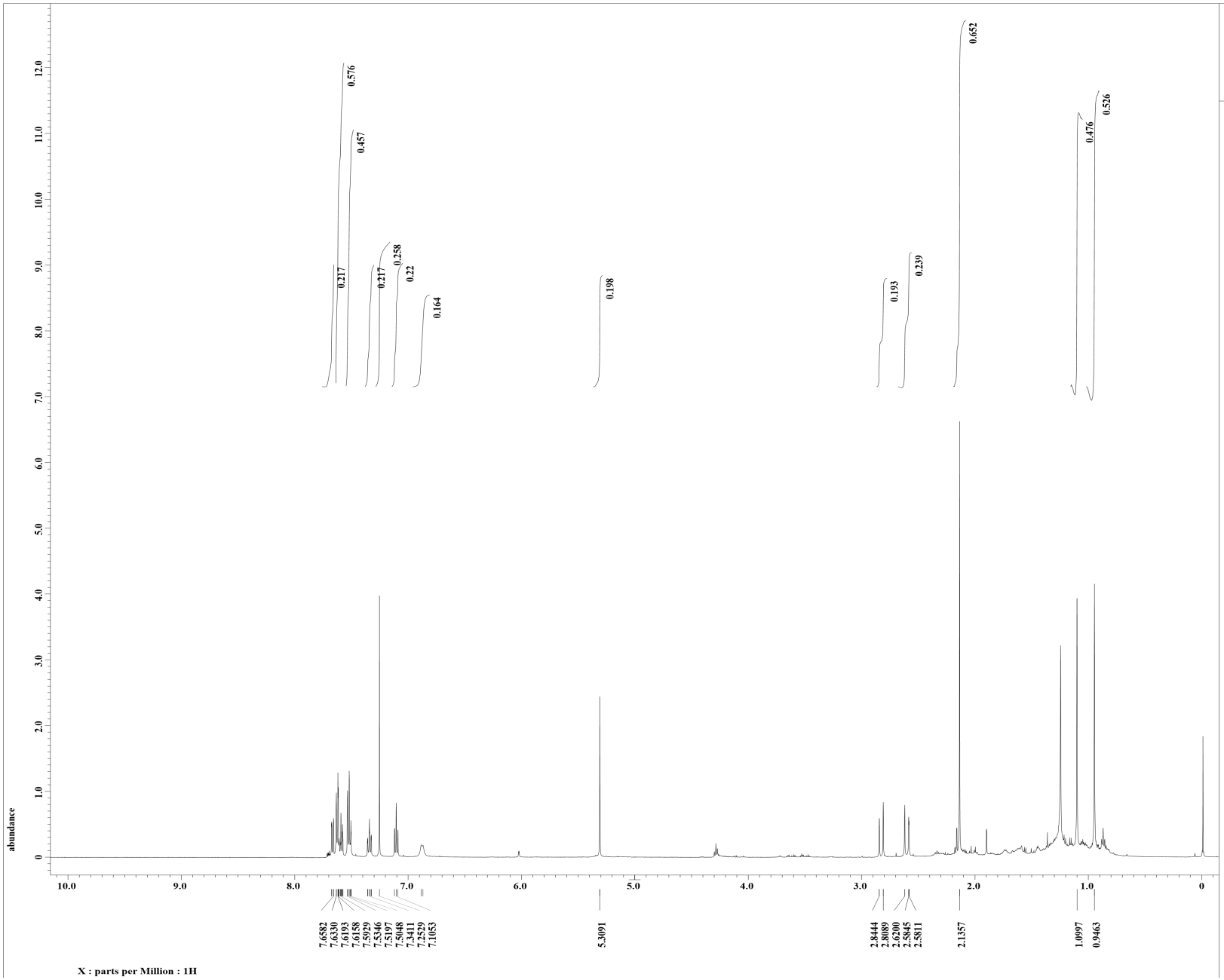
Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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             = 1357
Total_scans       = 1357

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          = 24.3[dC]
```



3gf



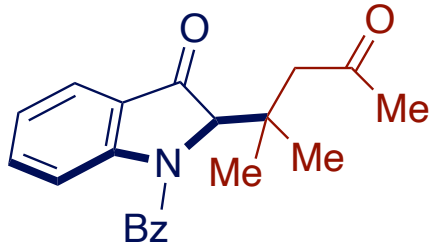
JEOL

```
Filename          = Bz-acetone-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#710413
Solvent           = CHLOROFORM-D
Creation_time     = 21-FEB-2020 18:47:21
Revision_time     = 21-FEB-2020 19:54:34
Current_time      = 21-FEB-2020 19:54:51

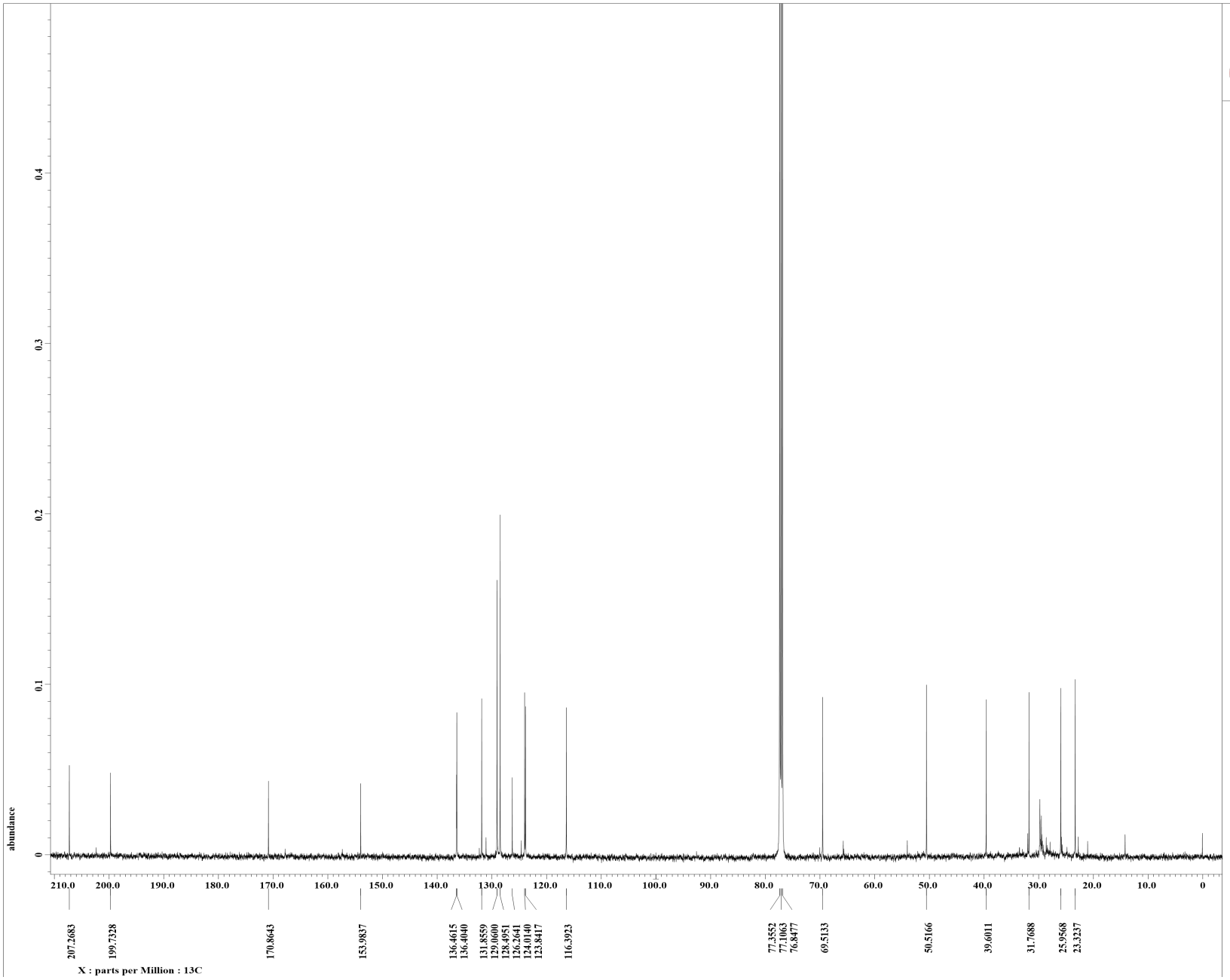
Content           = Bz-acetone-1H
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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          = 23.8[dC]
```



3jf

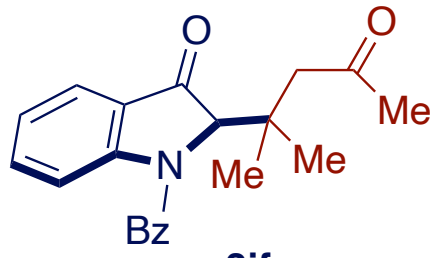


```
Filename          = Bz-acetone-5.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#713394
Solvent           = CHLOROFORM-D
Creation_time     = 22-FEB-2020 05:47:22
Revision_time     = 22-FEB-2020 13:52:57
Current_time      = 22-FEB-2020 13:54:27

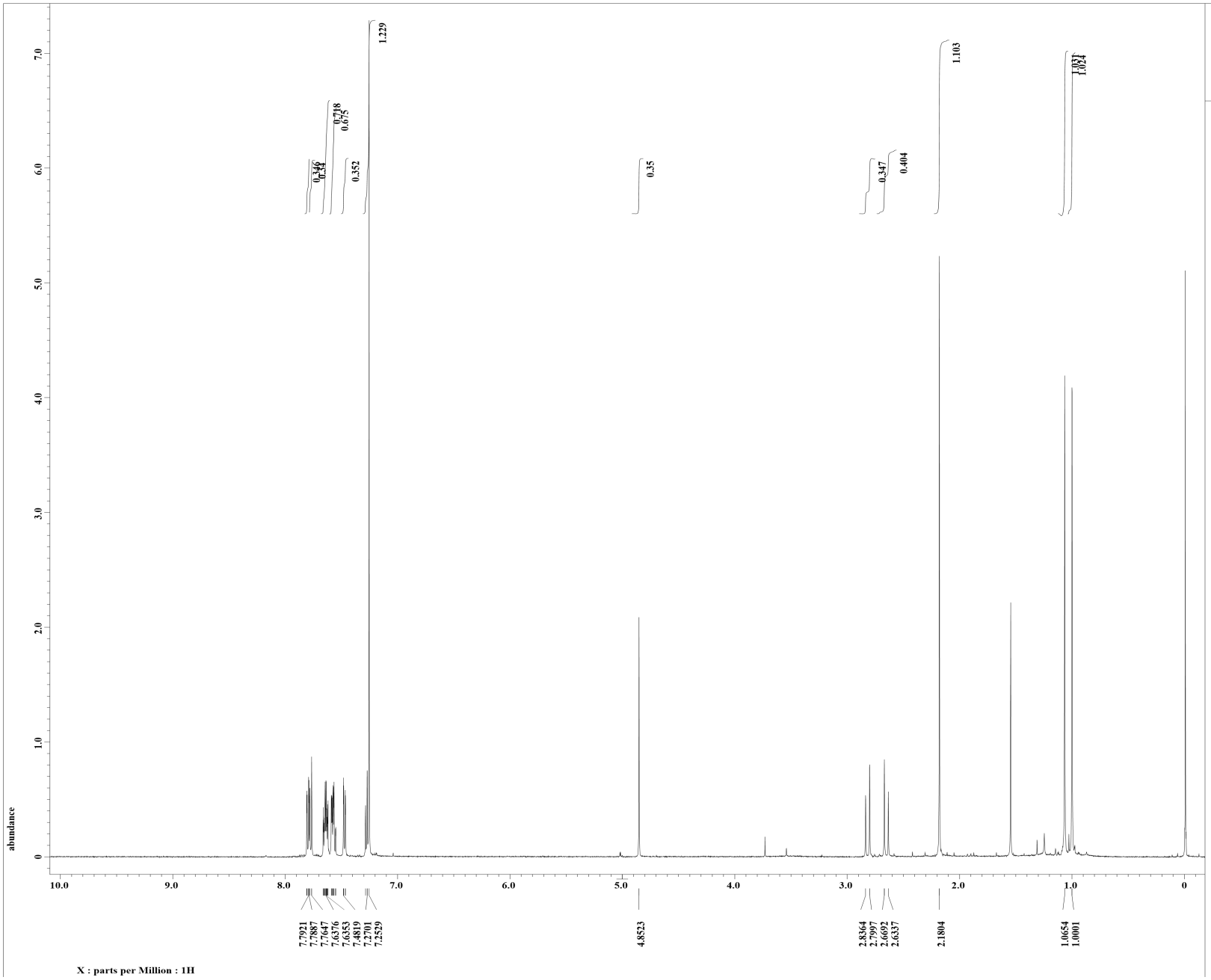
Content           = Bz-acetone-13C
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

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             = 13862
Total_scans       = 13862

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]
```



3jf

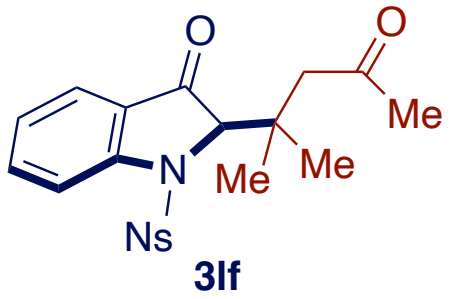



```
Filename          = 2Ns-acetone-1H-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#607091
Solvent           = CHLOROFORM-D
Creation_time     = 26-FEB-2020 15:53:59
Revision_time     = 26-FEB-2020 16:59:49
Current_time      = 26-FEB-2020 17:00:07

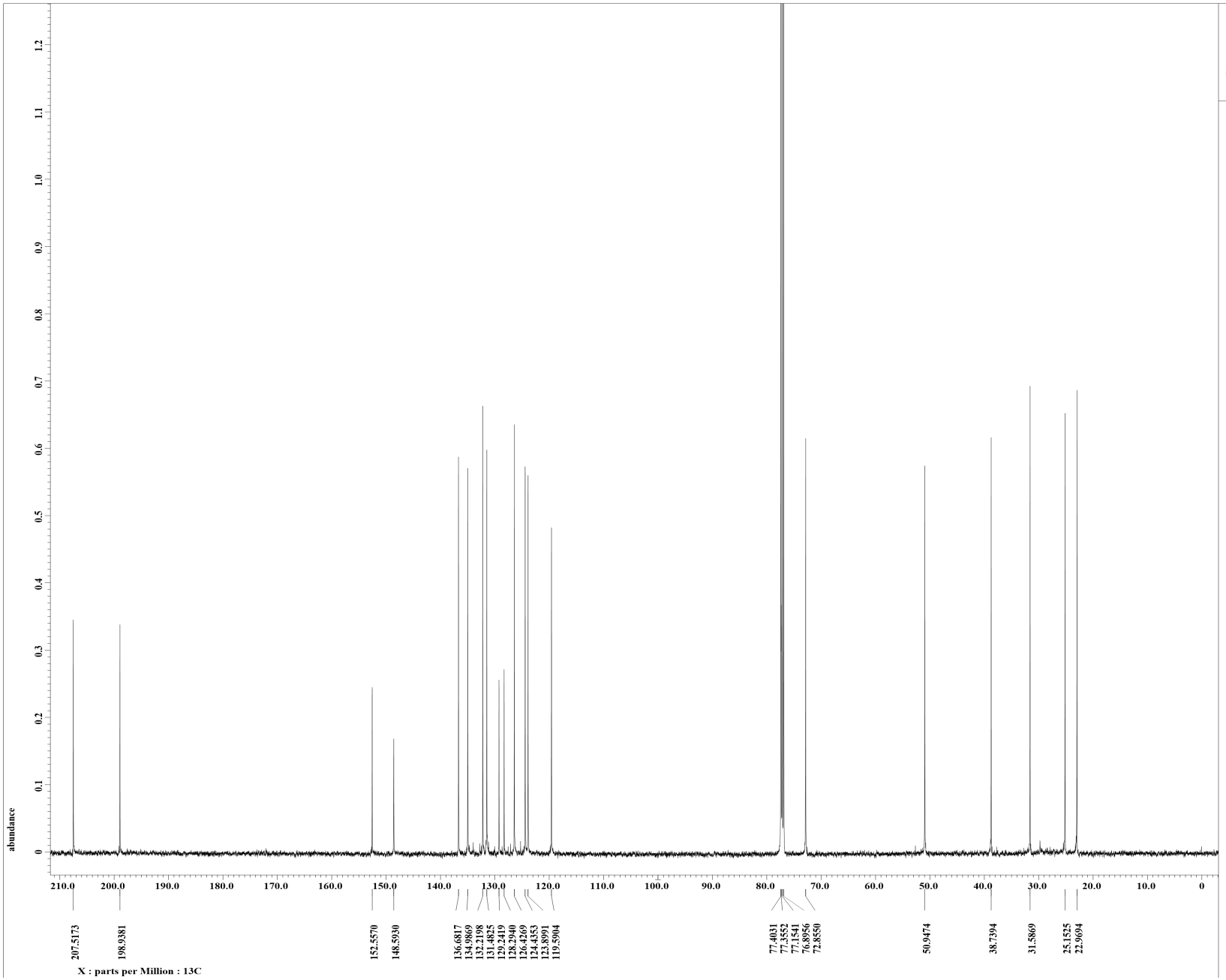
Content           = 2Ns-acetone-1H
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

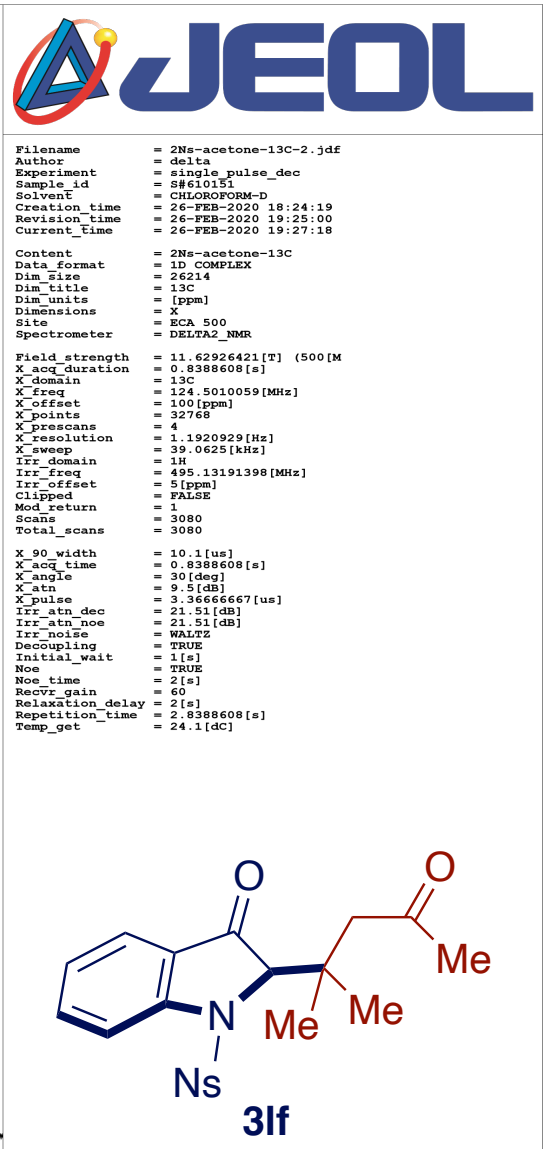
Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 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          = 23.4[dC]
```



3lf


abundance
X : parts per Million : 13C
207.5173
198.9381
152.5570
148.5930
136.6817
134.9869
132.2198
131.4825
129.2419
128.2940
126.4269
124.4353
123.8991
119.5904
77.4031
77.3552
77.1541
76.8956
72.8550
50.9474
38.7394
31.5869
25.1525
22.9694


Filename = 2Ns-acetone-13C-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#610151
Solvent = CHLOROFORM-D
Creation_time = 26-FEB-2020 18:24:19
Revision_time = 26-FEB-2020 19:25:00
Current_time = 26-FEB-2020 19:27:18
Content = 2Ns-acetone-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 = 3080
Total_scans = 3080
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]

O
O
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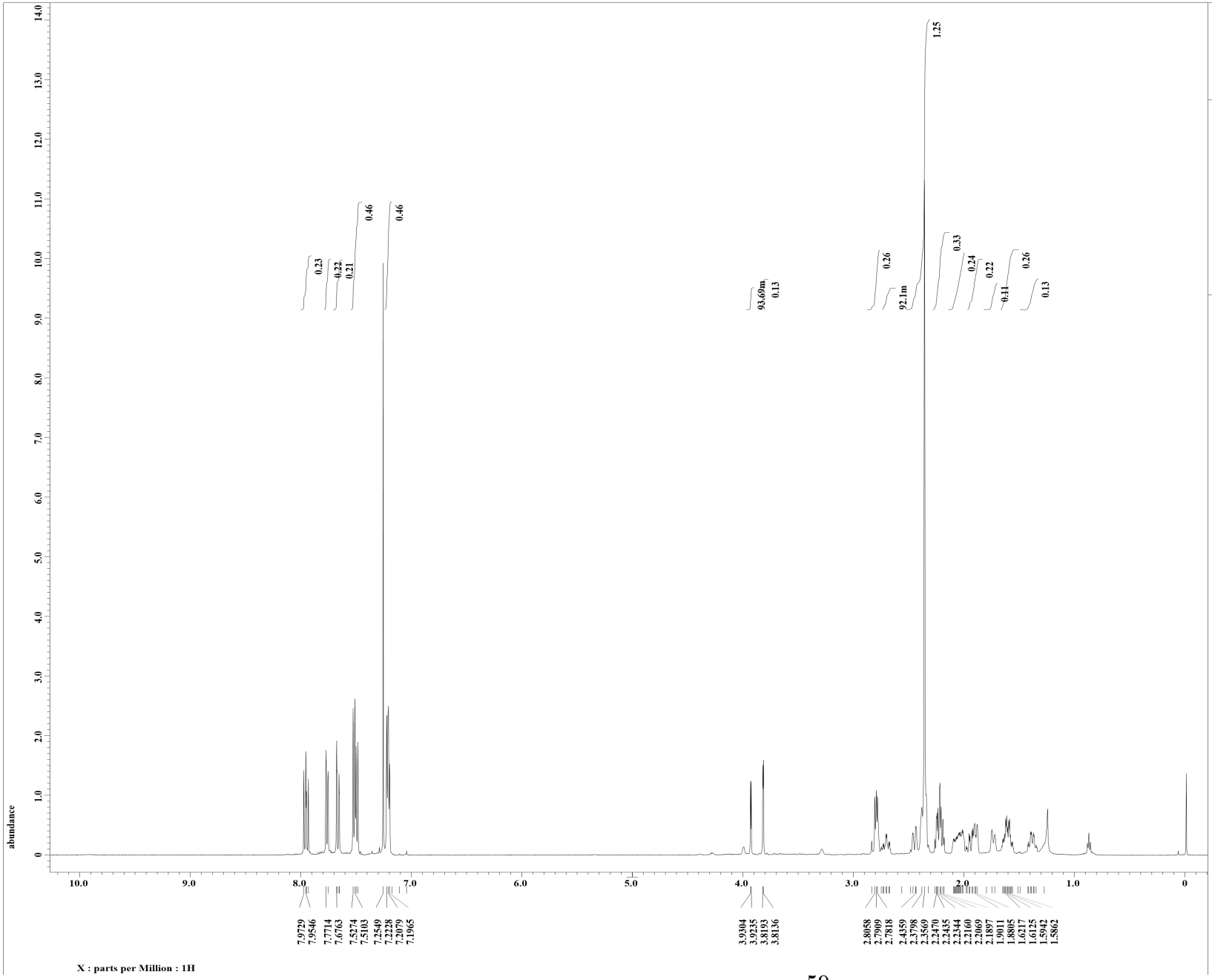
N
Me
Me
Ns

3lf



---- 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

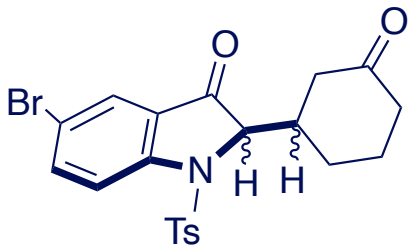
Derived from: TA2020-0318-2.jdf

Filename = TA2020-0318-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#302374
Solvent = CHLOROFORM-D
Creation_time = 3-JUN-2000 10:10:54
Revision_time = 18-MAR-2020 08:33:19
Current_time = 18-MAR-2020 08:33:49

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 = 23.2[dC]



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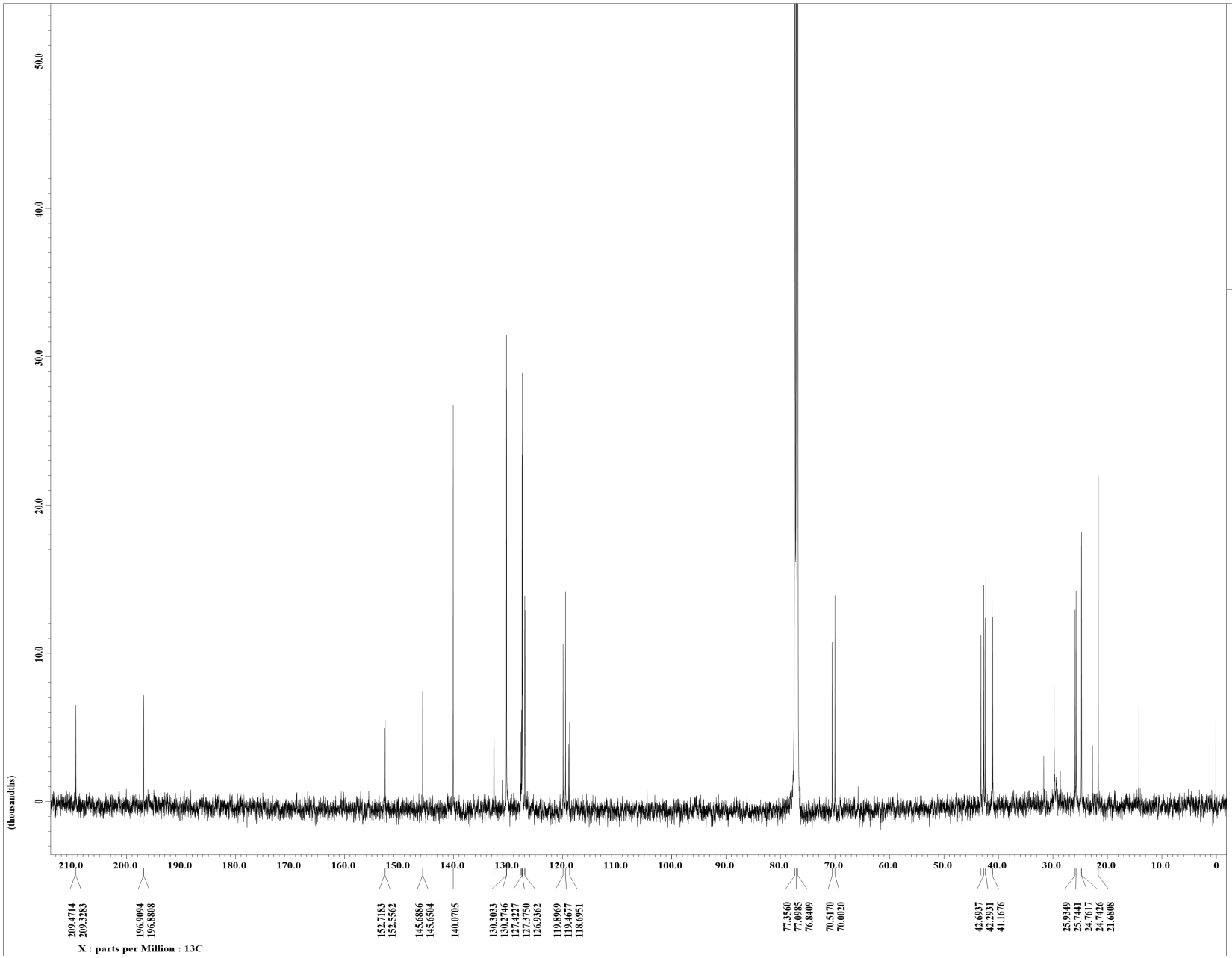



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

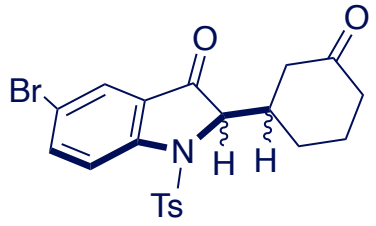
Derived from: R=5Br-cyclohexenone-C2-alk
```

```
Filename          = R=5Br-cyclohexenone-C
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#641217
Solvent           = CHLOROFORM-D
Creation_time     =  3-JUN-2000 09:59:29
Revision_time     = 18-MAR-2020 08:25:54
Current_time      = 18-MAR-2020 08:27:44

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             = 18301
Total_scans       = 18301

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          = 23.8[dC]
```



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