

Electronic Supplementary Information

Total Synthesis of (-)-20-Epiuleine via Stereocontrolled One-pot Asymmetric Azaelectrocyclization Followed by Novel 1,4-Addition Reaction

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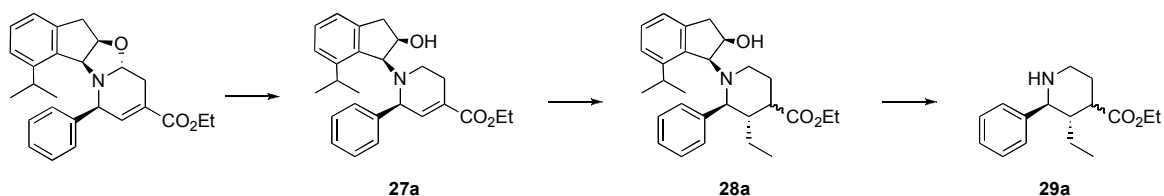
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General Procedure

All commercially available reagents were used without further purification. All solvents were used after distillation. Tetrahydrofuran, diethyl ether and toluene were refluxed over and distilled from sodium. Dichloromethane was refluxed over and distilled from P_2O_5 . Dimethylformamide (DMF) was distilled from CaH_2 . Preparative separation was usually performed by column chromatography on silica gel. The 1H NMR and ^{13}C NMR spectra were recorded using a 400 MHz spectrometer, and chemical shifts were represented as δ -values relative to the internal standard TMS. The IR spectra were recorded by a FT-IR spectrometer. The high-resolution mass spectra (HRMS) were measured by a ESI-TOF MS.



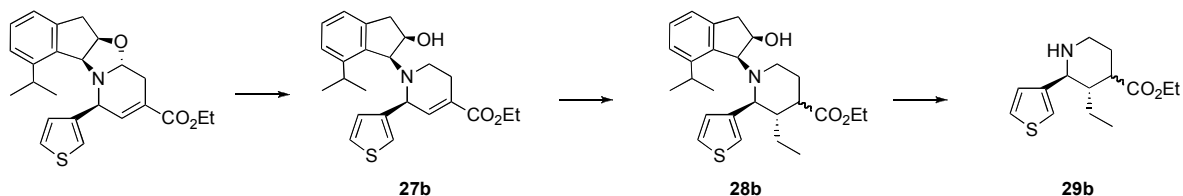
Ethyl (2S)-1-[(1S,2R)-2-hydroxyl-7-isopropylindan-1-yl]-2-phenyl-1,2,5,6-tetrahydropyridine-4-carboxylate (27a)

To a solution of aminoacetal (359 mg, 0.616 mmol) in THF (6 ml) were added sodium borohydride (114 mg, 3.01 mmol) and a trifluoroborane etherate complex (0.076 ml, 0.616 mmol) at 0 °C. After the mixture was stirred at 0 °C for 30 min, H_2O was added, and the resulting mixture was extracted with ether. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo* to give the alcohol product **27a** (81 mg, 90%) as yellow amorphous: IR (neat, cm^{-1}) 2959, 2360, 1690, 1238, 1087, 697; 1H NMR (400 MHz, $CDCl_3$, 50 °C) δ 7.06-7.34 (m, 7H), 6.81-6.92 (br s, 1H), 6.70-6.81 (br s, 1H), 4.73-5.15 (br s, 1H), 4.41-4.58 (br s, 1H), 4.28 (d, 1H, $J = 6.6$ Hz), 4.14-4.24 (m, 2H), 2.87-3.13 (br s, 4H), 2.38-2.74 (br m, 3H), 1.27 (t, 3H, $J = 7.1$ Hz), 1.14-1.24 (br s, 3H), 0.80-1.00 (br s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 50 °C) δ 166.9, 147.7, 140.6, 129.4, 1289.0, 128.3, 127.8, 123.4, 122.1, 60.8, 41.2, 26.2, 24.4, 22.9, 14.2, 5.1; ESI HRMS m/z calcd for $C_{26}H_{31}N_1O_3$ (M+Na) $^+$ 428.2202, found 428.2213.

Ethyl (2S,3S)-(-)-3-ethyl-2-phenylpiperidine-4-carboxylate (29a):

To a solution of **27a** (100 mg, 0.247 mmol) in ether (2.5 ml) was slowly added ethyl magnesium bromide (4.9 ml, 4.9 mmol, 1.0 M in ether) at 0 °C. After the mixture was stirred for 20 min, H_2O and a 1 N HCl solution were carefully added, and the resulting mixture was extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo* to give the crude **28a**.

To a solution of the crude piperidine and *n*-propylamine (0.18 ml, 2.22 mmol) in chloroform (2.5 ml) was added lead tetraacetate (438 mg, 0.99 mmol) at -50 °C. After the mixture was stirred for 15 min, it was added to an ice-1N aqueous NaOH solution. The resulting mixture was filtered, and extracted with chloroform. The organic layers were combined, washed with water, dried over $MgSO_4$, filtered and concentrated *in vacuo* to give the crude products. Column chromatography on silica gel (from 0% to 1.2% methanol in chloroform) gave **29a** (53 mg, 82% for 2 steps) in a 2.7 : 1 (0.73 : 0.27) mixture of C2 β and C2 α stereoisomers as a yellow amorphous solid: IR (neat, cm^{-1}) 2937, 1726, 1455, 1156, 753, 701; 1H NMR (400 MHz, $CDCl_3$) δ 7.24-7.38 (m, 5H), 4.05-4.23 (m, 2.27H), 3.40 (d, 0.73H, $J = 10.3$ Hz), 3.14-3.25 (m, 1H), 3.00 (dd, 0.27H, $J = 4.4$, 3.9 Hz), 2.95 (ddd, 0.27H, $J = 11.9$, 11.9, 3.4 Hz), 2.74-2.82 (m, 0.73H), 2.43-2.51 (m, 0.73H), 1.82-2.02 (m, 3H), 1.00-1.31 (m, 5H), 0.73 (t, 0.81H, $J = 7.3$ Hz), 0.67 (t, 2.19H, $J = 7.6$ Hz); major isomer ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.3, 142.9, 128.4, 127.9, 127.5, 65.1, 60.2, 47.0, 43.8, 30.3, 22.6, 14.2, 9.4; minor isomer ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4, 143.7, 128.3, 127.8, 127.2, 61.8, 59.8, 45.3, 42.4, 40.2, 28.9, 22.3, 14.3, 11.5; ESI HRMS m/z calcd for $C_{16}H_{23}N_1O_2$ (M+H) $^+$ 262.1807, found 262.1795.



Ethyl (2S)-1-[(1S,2R)-2-hydroxyl-7-isopropylindan-1-yl]-2-(thiophen-3-yl)-1,2,5,6-tetrahydropyridine-4-carboxylate (27b):

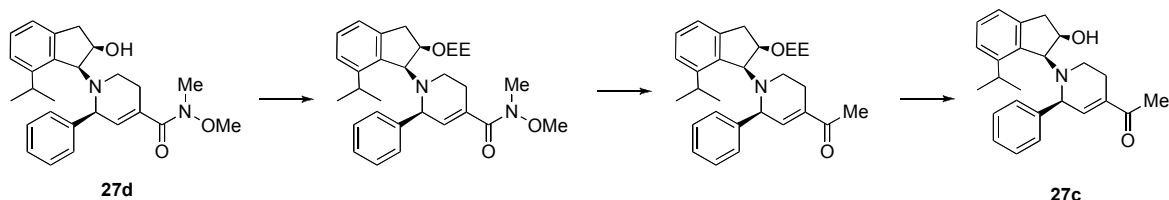
To a solution of aminoacetal derivative of thiophene (449 mg, 1.10 mmol) in acetonitrile (11 ml) were added sodium cyanoborohydride (344 mg, 5.48 mmol) and a 2 N HCl solution at 0 °C. After the mixture was stirred at 0 °C for 30 min, a saturated aqueous $NaHCO_3$ solution was added, and the resulting mixture was extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo* to give the crude products. Column chromatography on silica gel (from 9.1% to 25% ethyl acetate in hexane) gave **27b** (421 mg, 93%) as a yellow amorphous solid: IR (KBr disk, cm^{-1}) 2956, 2360, 1690, 1252, 775; 1H NMR (400 MHz, $CDCl_3$, 50 °C) δ 7.24-7.31 (br s, 1H), 7.19 (dd, 1H, $J = 7.6$, 7.6 Hz), 6.88-7.10 (m, 4H), 6.80 (s, 1H), 4.78-5.04 (br s, 1H), 4.35 (d, 1H, $J = 6.6$ Hz), 4.14-4.26 (m, 2H), 2.65-3.07 (br m, 3H), 2.80-2.48 (br m, 4H), 1.28 (t, 3H, $J = 7.1$ Hz), 1.05-1.18 (br d, 3H, $J = 5.3$ Hz), 0.80-0.97 (br d, 1H, $J =$

5.3 Hz); ^{13}C NMR (100 MHz, CDCl_3 , 50 $^\circ\text{C}$) δ 166.8, 147.6, 139.8, 129.1, 128.3, 125.7, 124.0, 123.3, 122.1, 60.5, 41.0, 26.2, 24.8, 22.8, 14.2, 7.1; ESI HRMS m/z calcd for $\text{C}_{24}\text{H}_{29}\text{N}_1\text{O}_3\text{S}_1$ ($\text{M}+\text{Na}$) $^+$ 434.1766, found 434.1767.

Ethyl (2*S*,3*S*)-(-)-3-ethyl-2-(thiophen-3-yl)-piperidine-4-carboxylate (**29b**):

To a solution of **27b** (100 mg, 0.242 mmol) in ether (2.5 ml) was slowly added ethyl magnesium bromide (4.9 ml, 4.9 mmol, 1.0 M in ether) at 0 $^\circ\text{C}$. After the mixture was stirred for 20 min, H_2O and a 1 N HCl solution were carefully added, and the resulting mixture was extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over MgSO_4 , filtered and concentrated *in vacuo* to give the crude **28b**.

To a solution of crude piperidine and *n*-propylamine (0.18 ml, 2.19 mmol) in chloroform (12 ml) was added lead tetraacetate (431 mg, 0.97 mmol) at -50 $^\circ\text{C}$. After the mixture was stirred for 15 min, it was added to an ice-1N aqueous sodium hydroxide solution. The resulting mixture was filtered, and extracted with chloroform. The organic layers were combined, washed with water, dried over MgSO_4 , filtered and concentrated *in vacuo* to give the crude products. Column chromatography on silica gel (from 0% to 1.3% methanol in chloroform) gave **29b** (53 mg, 75% for 2 steps) in a 3.8 : 1 (0.79 : 0.21) mixture of C2 β and C2 α stereoisomers as a yellow amorphous solid: IR (KBr disk, cm^{-1}) 3424, 2964, 2932, 2361, 2344, 1719, 1157, 756; ^1H NMR (400 MHz, CDCl_3) δ 7.24-7.29 (m, 1H), 7.25-7.20 (m, 1H), 7.10-7.14 (m, 1H), 4.08-4.26 (m, 2.21H), 3.57 (d, 0.79H, J = 10.3 Hz), 3.06-3.20 (m, 1H), 2.86-2.99 (m, 0.42H), 2.75 (ddd, 0.79H, J = 11.4, 11.4, 3.7 Hz), 2.44 (ddd, 0.79H, J = 11.2, 11.2, 4.8 Hz), 1.74-1.94 (m, 3H), 1.06-1.34 (m, 5H) 0.78 (t, 3H, J = 7.6 Hz), 0.68 (t, 3H, J = 7.6 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 175.1, 143.9, 126.6, 125.6, 125.5, 121.8, 60.2, 60.1, 46.9, 46.2, 44.1, 30.1, 22.8, 14.1, 9.4; representative signals of minor isomer in its ^{13}C NMR (100 MHz, CDCl_3) δ 174.4, 144.9, 59.9, 56.7, 44.9, 42.0, 40.2, 28.0, 22.2, 14.2, 11.6; ESI HRMS m/z calcd for $\text{C}_{14}\text{H}_{21}\text{N}_1\text{O}_2\text{S}_1$ ($\text{M}+\text{H}$) $^+$ 268.1371, found 268.1358.

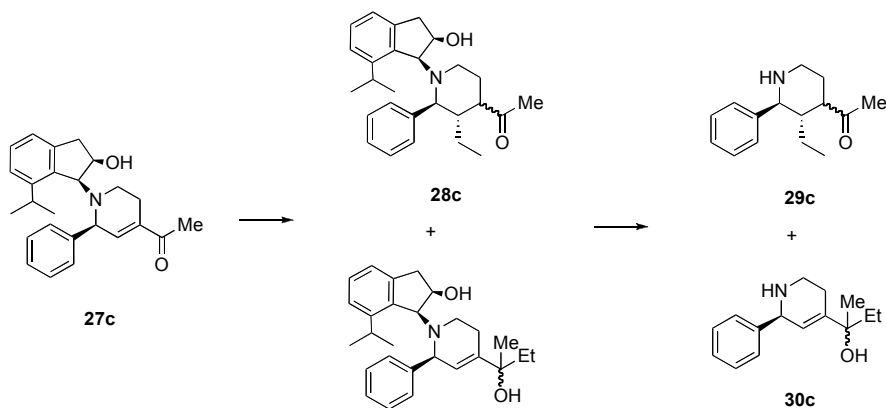


(1*S*,2*R*)-*cis*-1-[(2*S*)-4-Acetyl-2-phenyl-1,2,5,6-tetrahydropyridin-1-yl]-7-isopropylindan-2-ol (**27c**)

To a solution of **27d** (155 mg, 0.369 mmol) in dichloromethane (1.8 ml) were added ethyl vinyl ether (0.176 ml, 1.843 ml) and PPTS (9 mg, 0.0369 mmol) at room temperature. After the mixture was stirred at reflux for 20 h, a saturated aqueous NH_4Cl solution was added, and the resulting mixture was extracted with chloroform. The organic layers were combined, washed with brine, dried over MgSO_4 , filtered and concentrated *in vacuo* to give the ethoxyethyl protected alcohol product (153 mg, 85%) as a yellow amorphous solid.

To a solution of ethoxyethyl protected alcohol (634 mg, 1.286 mmol) in THF (12.8 ml) was added methyl magnesium chloride (1.72 ml, 5.147 mmol) at 0 $^\circ\text{C}$. After the mixture was stirred at 0 $^\circ\text{C}$ for 30 min, then added to H_2O , the resulting mixture was extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over MgSO_4 , filtered and concentrated *in vacuo* to give the ketone product (539 mg, 94%) as a white amorphous solid.

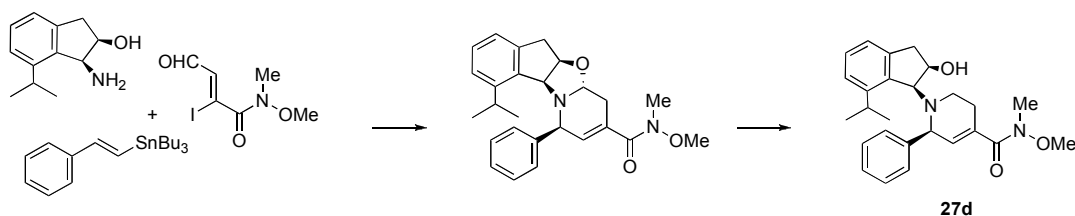
To a solution of the ketone (124 mg, 0.277 mmol) in MeOH (2.8 ml) was added a 2 N HCl solution (2.8 ml) at room temperature. After the mixture was stirred at room temperature for 28 h, a saturated aqueous NaHCO_3 solution was added, and the resulting mixture was extracted with chloroform. The organic layers were combined, washed with brine, dried over MgSO_4 , filtered and concentrated *in vacuo* to give **27c** (100 mg, 96%) as a white amorphous solid: IR (KBr disk, cm^{-1}) 3457, 2960, 2940, 1650, 1267, 1088; ^1H NMR (400 MHz, CDCl_3 , 50 $^\circ\text{C}$) δ 7.00-7.41 (m, 7H), 6.80-6.93 (br s, 1H), 6.58-6.67 (br s, 1H), 4.77-5.40 (br s, 1H), 4.42-4.60 (br s, 1H), 4.28 (d, 1H, J = 6.6 Hz), 2.85-3.12 (br s, 3H), 2.26-2.80 (br m, 4H), 2.25 (s, 3H), 1.10-1.30 (br m, 3H), 0.80-0.97 (br s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , 50 $^\circ\text{C}$) δ 198.4, 147.6, 141.7, 140.9, 136.8, 136.7, 129.3, 128.9, 128.4, 127.9, 123.4, 122.0, 62.7, 41.1, 29.0, 25.0, 24.9, 24.3, 23.3, 23.0, 15.2; ESI HRMS m/z calcd for $\text{C}_{25}\text{H}_{29}\text{N}_1\text{O}_2$ ($\text{M}+\text{Na}$) $^+$ 398.2096, found 398.2105.



(2*S*,3*S*)-4-Acetyl-3-ethyl-2-phenyl-piperidine (**29c**), and 2-[(2*S*)-2-phenyl-1,2,5,6-tetrahydropyridin-4-yl]-butan-2-ol (**30c**):

To a solution of **27c** (100 mg, 0.266 mmol) in ether (2.6 ml) was slowly added ethyl magnesium bromide (5.3 ml, 5.3 mmol, 1.0 M in ether) at 0 °C. After the mixture was stirred for 20 min, water was carefully added followed by 1 N hydrochloric acid, and extracted with ethyl acetate. The organic layers were washed with brine, dried over MgSO₄, filtered and concentrated *in vacuo* to give the crude product.

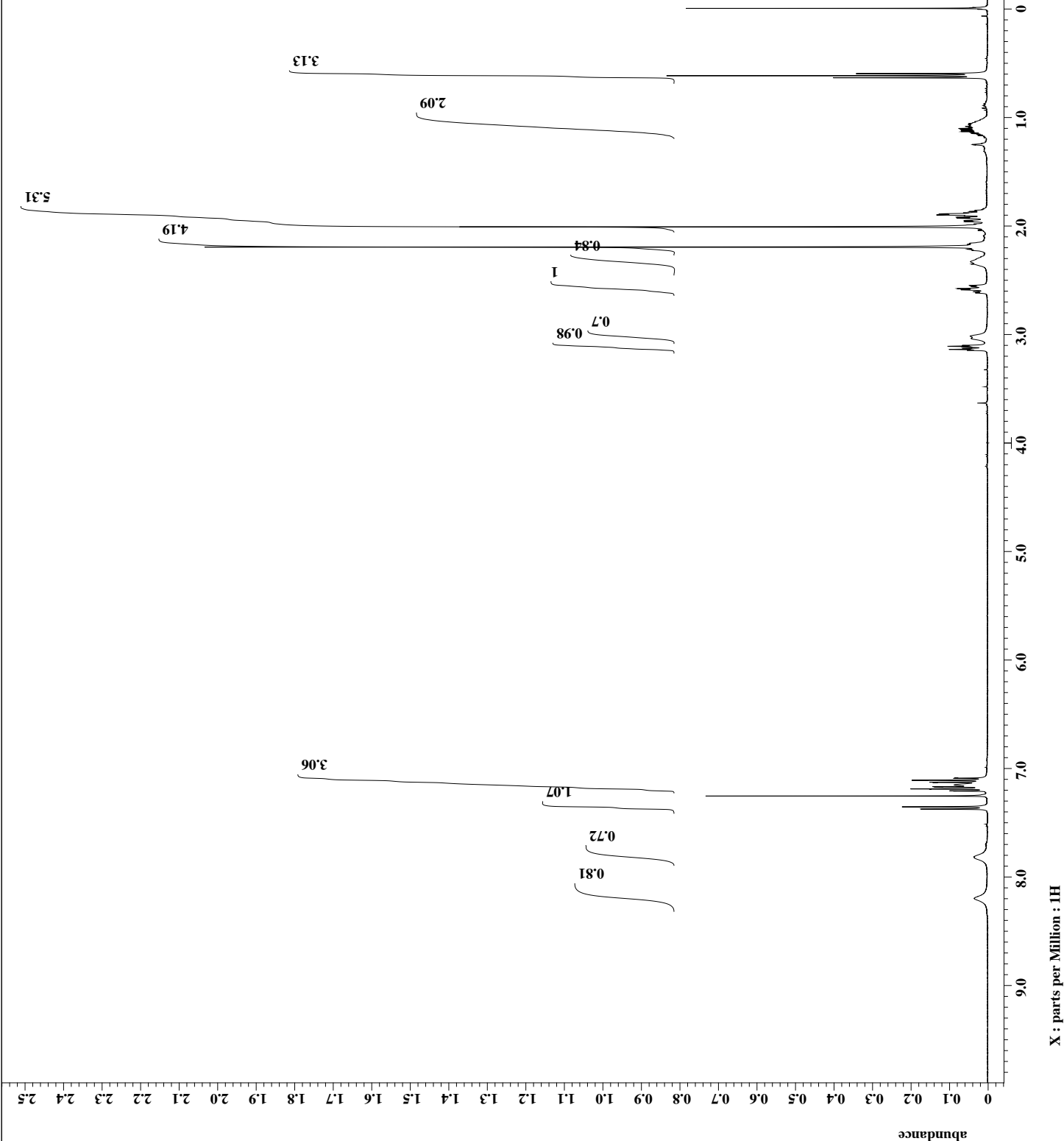
To a solution of the crude piperidine and *n*-propylamine (0.20 ml, 2.40 mmol) in chloroform (2.6 ml) was added lead tetraacetate (472 mg, 1.07 mmol) at -50 °C. After the mixture was stirred for 15 min, it was added to an ice-1N aqueous sodium hydroxide solution. The resulting mixture was filtered, and extracted with chloroform. The organic layers were combined, washed with water, dried over MgSO₄, filtered and concentrated *in vacuo* to give the crude products. Column chromatography on silica gel (from 0% to 1.2% methanol in chloroform) gave **29c** (53 mg, 41% for 2 steps) in a 2.2 : 1 (0.69 : 0.31) mixture of C2β and C2α stereoisomers as a yellow oil and **30c** (16 mg, 26%) in a 1:1 mixture of stereoisomers as a yellow oil. Data for **29c**: IR (KBr disk, cm⁻¹) 2960, 2360, 2340, 1709, 1354, 756; ¹H NMR (400 MHz, CDCl₃) δ 7.21-7.40 (m, 5H), 4.21 (d, 0.31H, *J* = 9.6 Hz), 3.39 (d, 0.69H, *J* = 10.1 Hz), 3.09-3.24 (m, 1H), 2.84-2.93 (m, 0.62H), 2.80 (ddd, 0.69H, *J* = 11.9, 11.7, 2.5 Hz), 2.59 (ddd, 0.69H, *J* = 11.4, 11.4, 3.6 Hz), 2.20 (s, 3H), 1.66-2.05 (m, 3H), 0.97-1.29 (m, 2H), 0.68 (t, 0.93H, *J* = 7.6 Hz), 0.62 (t, 2.07H, *J* = 7.6 Hz); major isomer ¹³C NMR (100 MHz, CDCl₃) δ 211.6, 142.7, 128.4, 127.9, 127.6, 65.1, 54.6, 46.7, 43.2, 29.9, 28.4, 22.5, 9.6; minor isomer ¹³C NMR (100 MHz, CDCl₃) δ 211.2, 143.6, 143.6, 128.3, 127.8, 127.2, 61.4, 45.4, 41.9, 30.5, 27.6, 21.7, 11.9; ESI HRMS *m/z* calcd for C₁₅H₂₁N₁O₁ (M+H)⁺ 232.1701, found 232.1690. Data for **30c**: IR (KBr disk, cm⁻¹) 3420, 2940, 2930, 1650, 1456, 760; ¹H NMR (400 MHz, CDCl₃) δ 7.36-7.22 (m, 5H), 5.78-5.72 (br m, 1H), 4.55-4.51 (br m, 1H), 3.19-3.09 (m, 1H), 2.97-2.88 (m, 1H), 2.30-2.12 (m, 2H), 1.68-1.58 (m, 2H), 1.34-1.30 (m, 3H), 0.91-0.82 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 7143.1, 142.4, 142.3, 128.5, 127.9, 127.9, 127.5, 127.0, 122.1, 121.7, 75.0, 58.4, 58.3, 42.0, 41.7, 32.9, 32.8, 27.1, 27.0, 24.9, 24.7, 8.3, 8.1; ESI HRMS *m/z* calcd for C₁₅H₂₁N₁O₁ (M+H)⁺ 232.1701, found 232.1700.



(2S)-1-[(1S,2R)-2-hydroxyl-7-isopropylindan-1-yl]-N-methoxy-N-methyl-2-phenyl-1,2,5,6-tetrahydropyridine-4-carboxamide (27d):

To a suspension of Weinreb amide (100 mg, 0.372 mmol) and molecular sieve 4A (372 mg) in DMF (2.0 ml) was added *cis*-1-amino-7-isopropylindan-2-ol (**9**) (75 mg, 0.390 mmol) at room temperature, and then the mixture was stirred for 10 min at this temperature. To this suspension were added lithium chloride (39 mg, 0.929 mmol), tri(2-furyl)phosphine (28 mg, 0.199 mmol) and tris(dibenzylideneacetone)dipalladium(0) (27 mg, 0.029 mmol) at room temperature, the mixture was stirred for 10 min at this temperature then a solution of phenylvinylstannane (219 mg, 0.558 mmol) in DMF (0.6 ml) was added to this suspension. After the reaction mixture was stirred at 80 °C for 3 h, a 10% aqueous NH₃ solution was added, and the resulting mixture was extracted with ether. The organic layers were combined, washed with brine, dried over MgSO₄, filtered and concentrated *in vacuo* to give the crude aminoacetal products. Column chromatography on silica gel (from 33% to 50% ethyl acetate in hexane) gave the aminoacetal (136 mg, 87%) as a yellow foam: IR (neat, cm⁻¹) 2960, 2360, 1620, 1161, 1021, 747; ¹H NMR (400 MHz, CDCl₃) δ 7.30-7.43 (m, 5H), 7.14 (dd, 1H, *J* = 7.6, 7.6 Hz), 6.94-7.01 (m, 2H), 6.16 (d, 1H, *J* = 1.6 Hz), 4.95-4.98 (m, 1H), 4.89 (d, 1H, *J* = 5.7 Hz), 4.46 (d, 1H, *J* = 5.0 Hz), 4.07-4.09 (m, 1H), 3.62 (s, 3H), 3.22 (s, 3H), 3.02-3.19 (m, 2H), 2.79-2.83 (m, 1H), 2.65-2.75 (m, 1H), 2.61 (qq, 1H, *J* = 6.9, 6.6 Hz), 0.99 (d, 3H, *J* = 6.6 Hz), 0.56 (d, 3H, *J* = 6.9 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 169.4, 147.8, 143.1, 142.1, 136.3, 132.0, 129.3, 128.7, 128.3, 127.8, 126.4, 123.4, 121.6, 86.5, 75.0, 74.3, 61.5, 61.2, 39.6, 33.8, 28.0, 26.7, 23.4, 22.8; ESI HRMS *m/z* calcd for C₂₆H₃₀N₂O₃ (M+Na)⁺ 441.2154, found 441.2153.

To a solution of the aminoacetal (136 mg, 0.323 mmol) in acetonitrile (3.2 ml) was added sodium cyanoborohydride (101 mg, 1.617 mmol) at 0 °C. After the mixture was stirred at 0 °C for 1 h, H₂O was added, and the resulting mixture was extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over MgSO₄, filtered and concentrated *in vacuo* to give the alcohol product **27d** (118 mg, 87%) as yellow amorphous solid: IR (neat, cm⁻¹) 2960, 2360, 1618, 1382, 1087, 703; ¹H NMR (400 MHz, CDCl₃, 50 °C) δ 7.00-7.51 (m, 7H), 6.74-6.92 (br s, 1H), 6.07-6.15 (br s, 1H), 4.38-4.57 (br s, 1H), 4.28 (d, 1H, *J* = 6.6 Hz), 3.58-3.65 (m, 4H), 2.86-3.30 (br m, 7H), 2.30-2.86 (br m, 3H), 1.16-1.32 (br s, 3H), 0.82-1.10 (br s, 3H); ¹³C NMR (100 MHz, CDCl₃, 50 °C) δ 170.5, 147.6, 141.4, 136.9, 134.3, 129.3, 129.1, 129.0, 128.7, 128.3, 127.7, 123.3, 122.1, 70.1, 63.8, 62.3, 61.2, 41.0, 33.6, 32.1, 28.0, 24.5, 22.9; ESI HRMS *m/z* calcd for C₂₆H₃₂N₂O₃ (M+Na)⁺ 443.2311, found 443.2307.



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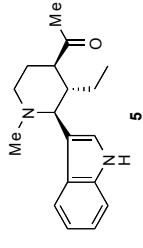
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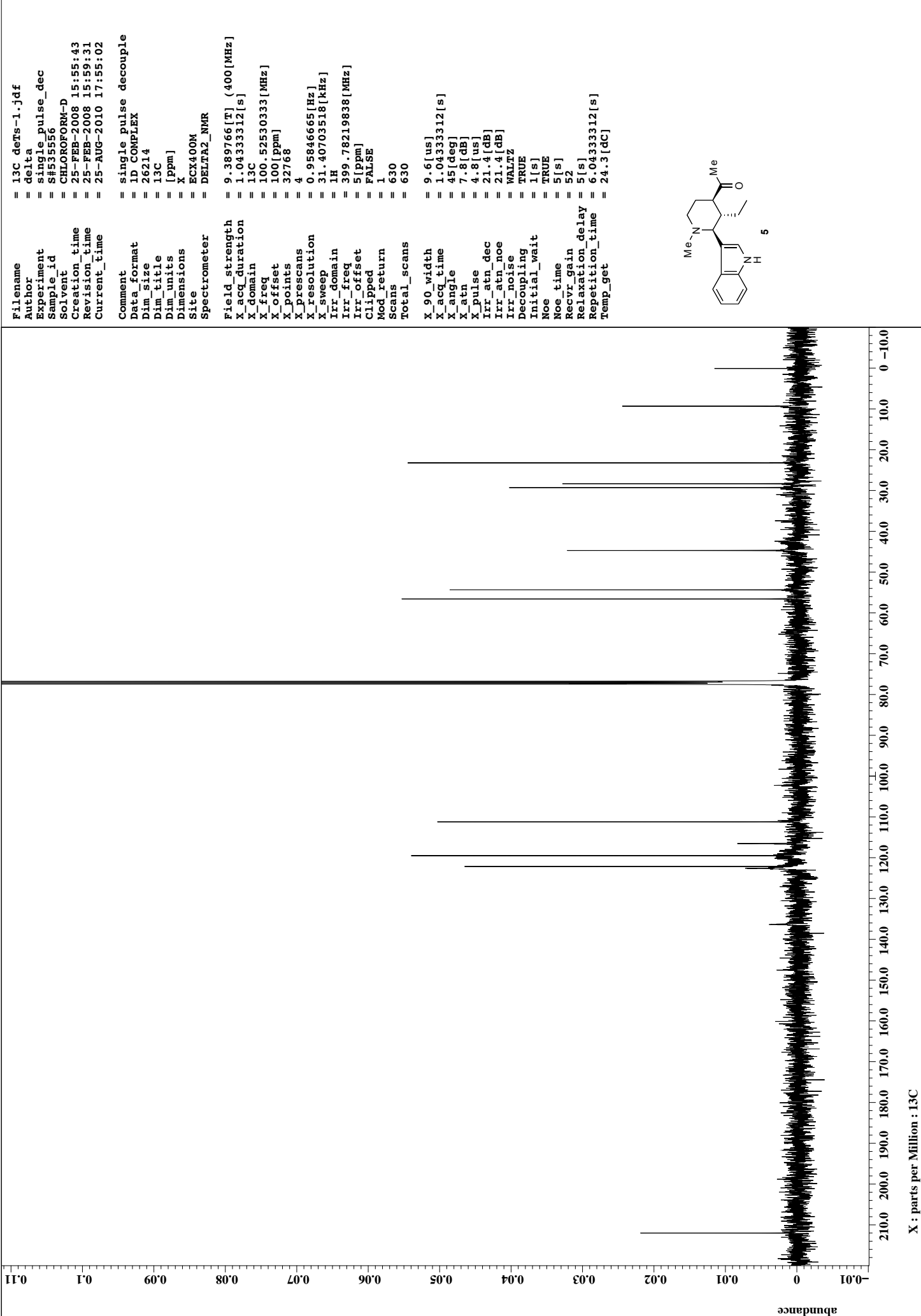
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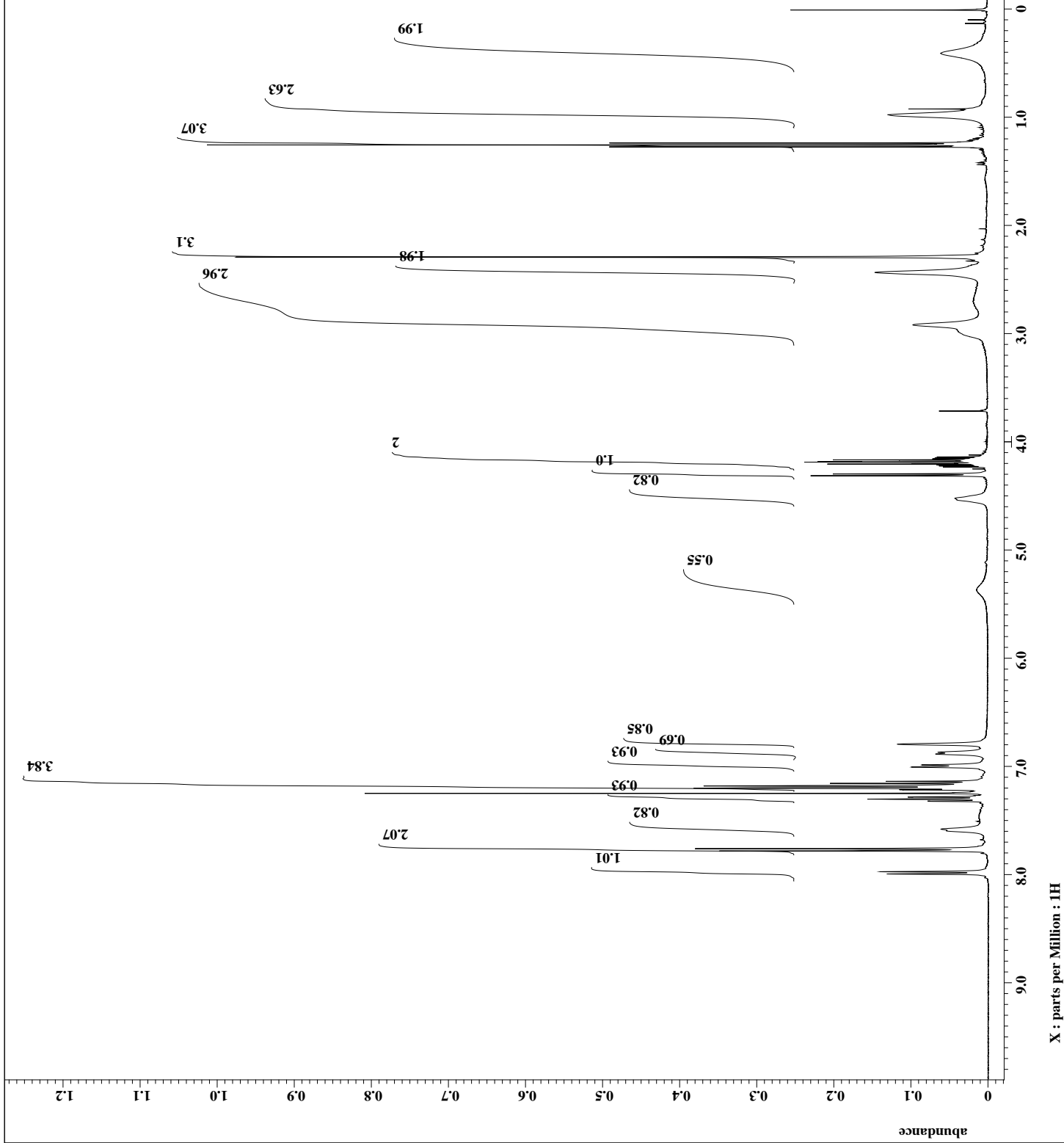
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Decoupling  = TRUE
Initial_wait = 1[s]
Noe         = TRUE
Noe_time    = 5[s]
Recvr_gain  = 52
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get    = 24.3[dc]

```

X : parts per Million : 13C



```

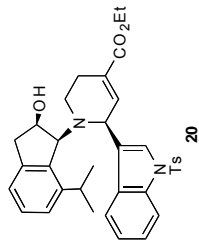
Filename = 1H NaBH4 55cC-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 9-FEB-2009 12:36:19
Revision_time = 6-NOV-2009 17:09:21
Current_time = 25-AUG-2010 17:12:35

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.5[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get = 55[dc]

```



```

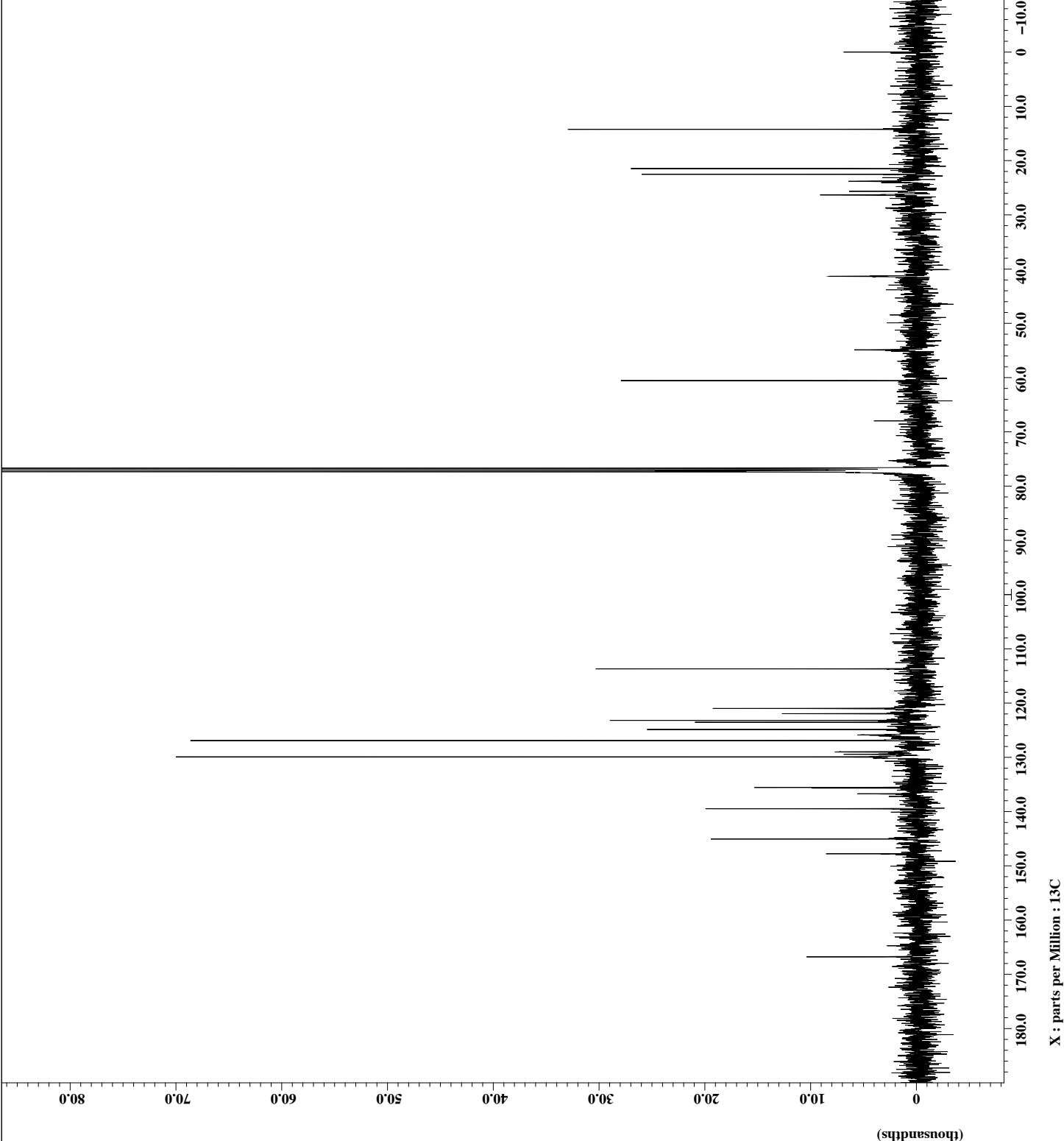
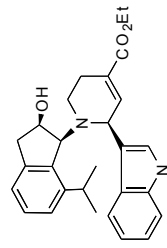
Filename = 13C NaBH4 500C-1.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#657632
Solvent = CHLOROFORM-D
Creation_time = 13-FEB-2008 18:58:09
Revision_time = 13-FEB-2008 19:01:10
Current_time = 25-AUG-2010 17:25:55

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

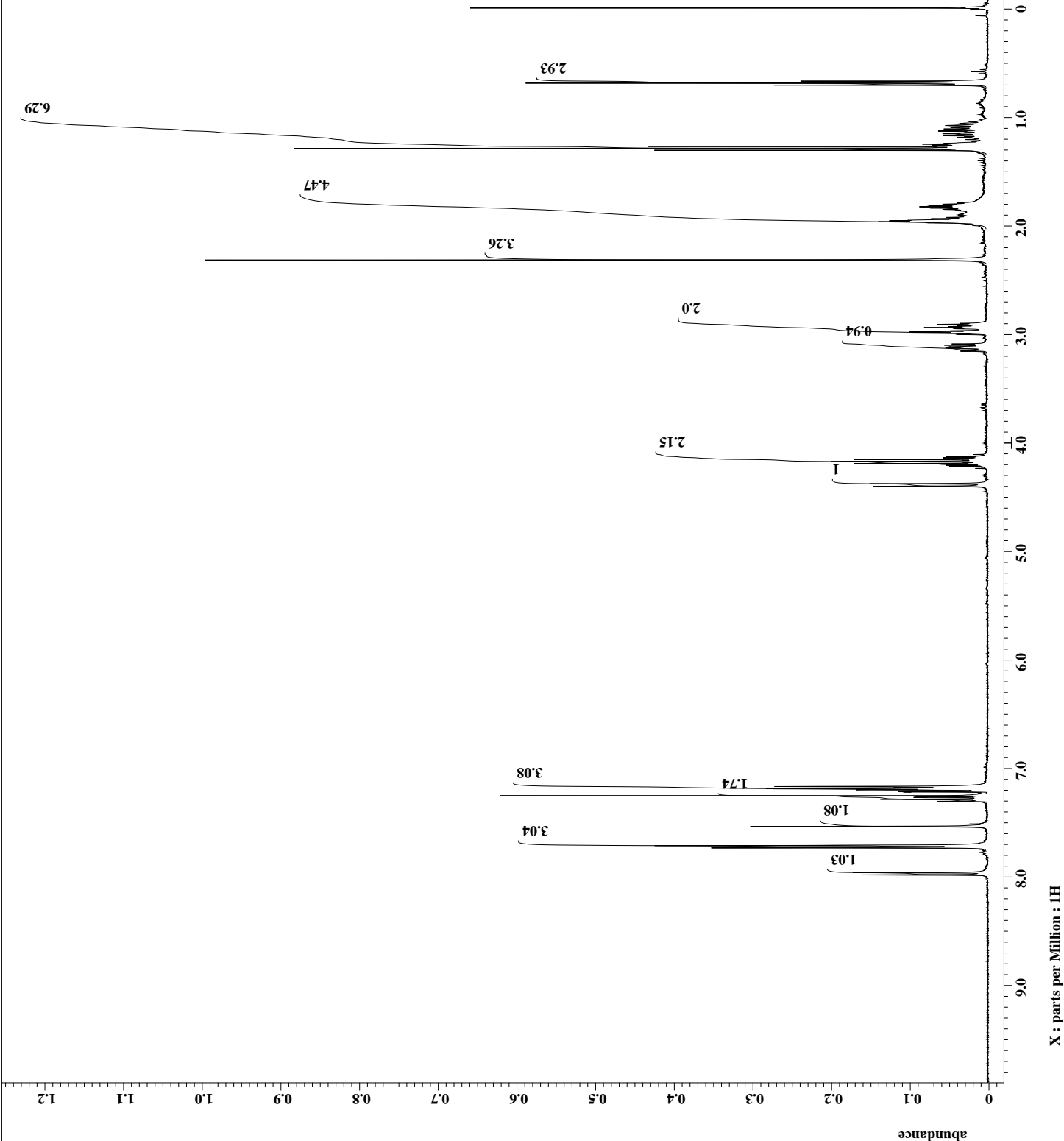
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 415
Total_scans = 415

X_90_width = 9.6[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 7.8[db]
x_pulse = 4.8[us]
Irr_atn_dec = 21.4[db]
Irr_atn_noe = 21.4[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 50[dc]

```



X : parts per Million : 13C



```

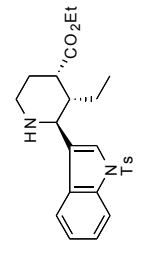
Filename = 1H NH isomer-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 9-FEB-2009 15:38:06
Revision_time = 24-AUG-2010 18:17:16
Current_time = 24-AUG-2010 18:17:38

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

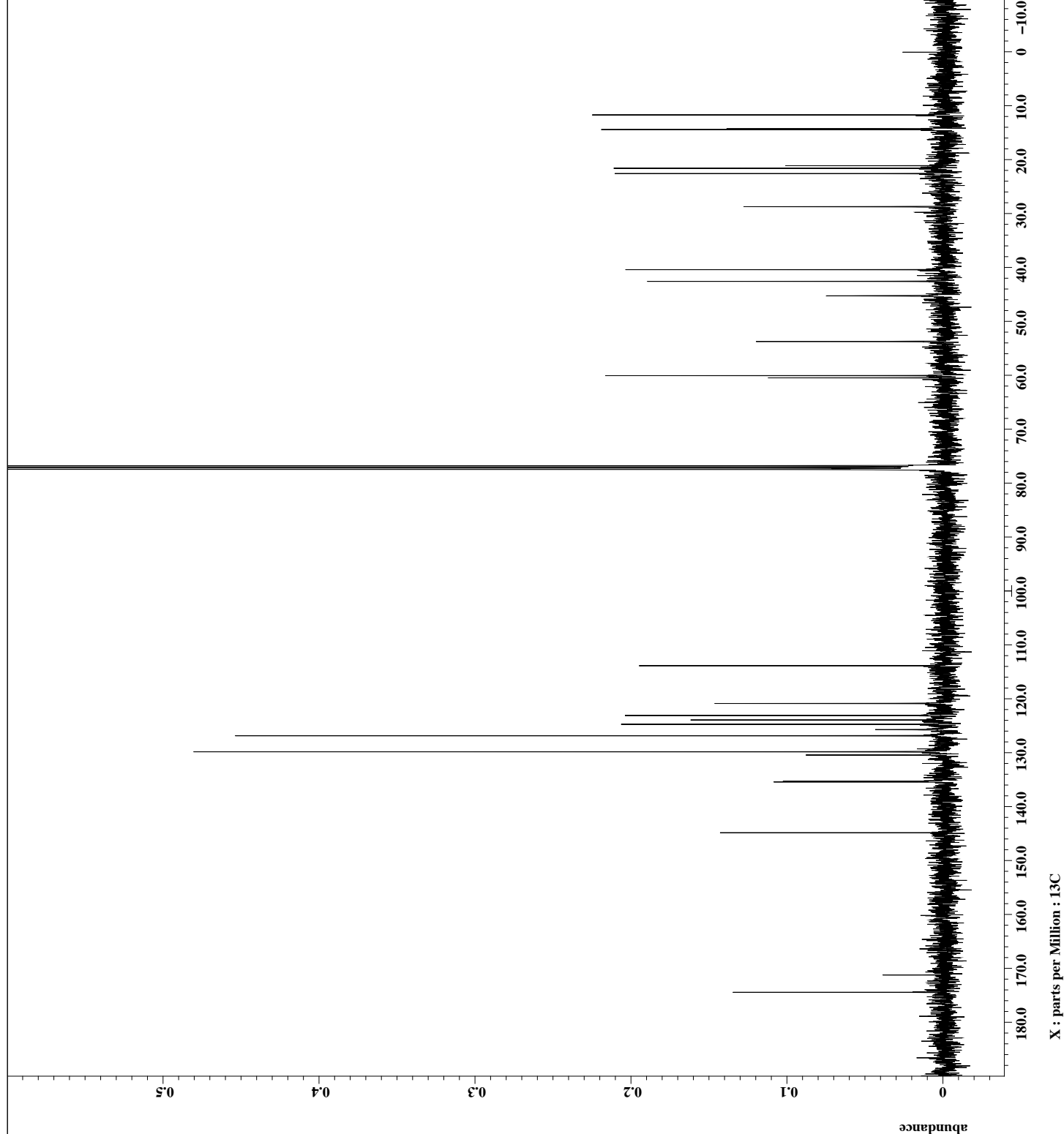
X_90_width = 10.5[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get = 23.7[dC]

```



22a

X : parts per Million : 1H



```

Filename = 13C NH isomer-1.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#511988
Solvent = CHLOROFORM-D
Creation_time = 18-FEB-2008 14:28:20
Revision_time = 18-FEB-2008 14:31:45
Current_time = 24-AUG-2010 18:18:35

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

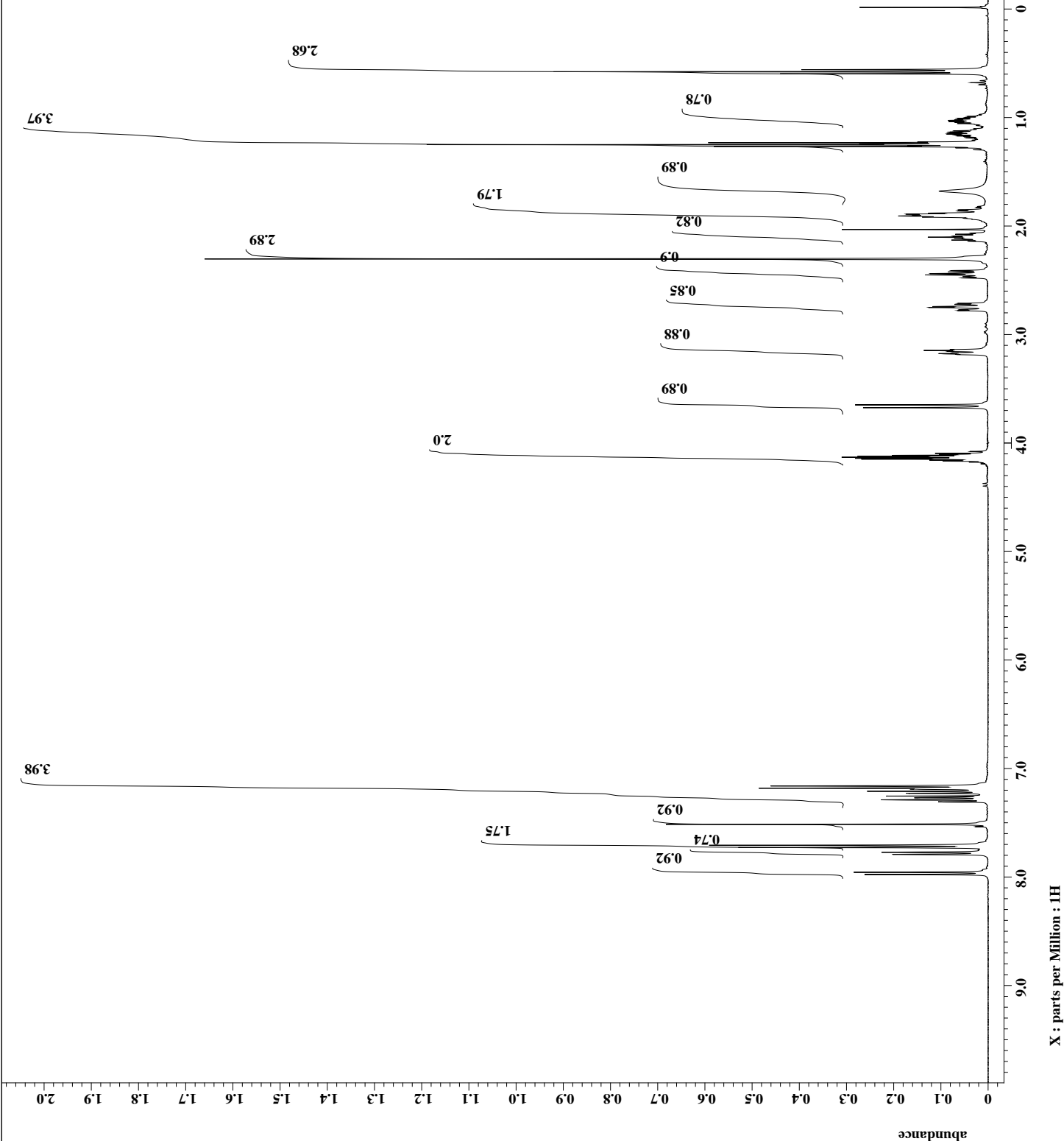
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 153
Total_scans = 153

X_90_width = 9.6[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 7.8[db]
x_pulse = 4.8[us]
Irr_atn_dec = 21.4[db]
Irr_atn_noe = 21.4[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 60
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.3[dc]

```

22a

X : parts per Million : 13C



```

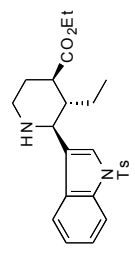
Filename = 1H NH-2.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 13-FEB-2008 12:07:25
Revision_time = 25-AUG-2010 17:26:41
Current_time = 25-AUG-2010 17:26:53

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

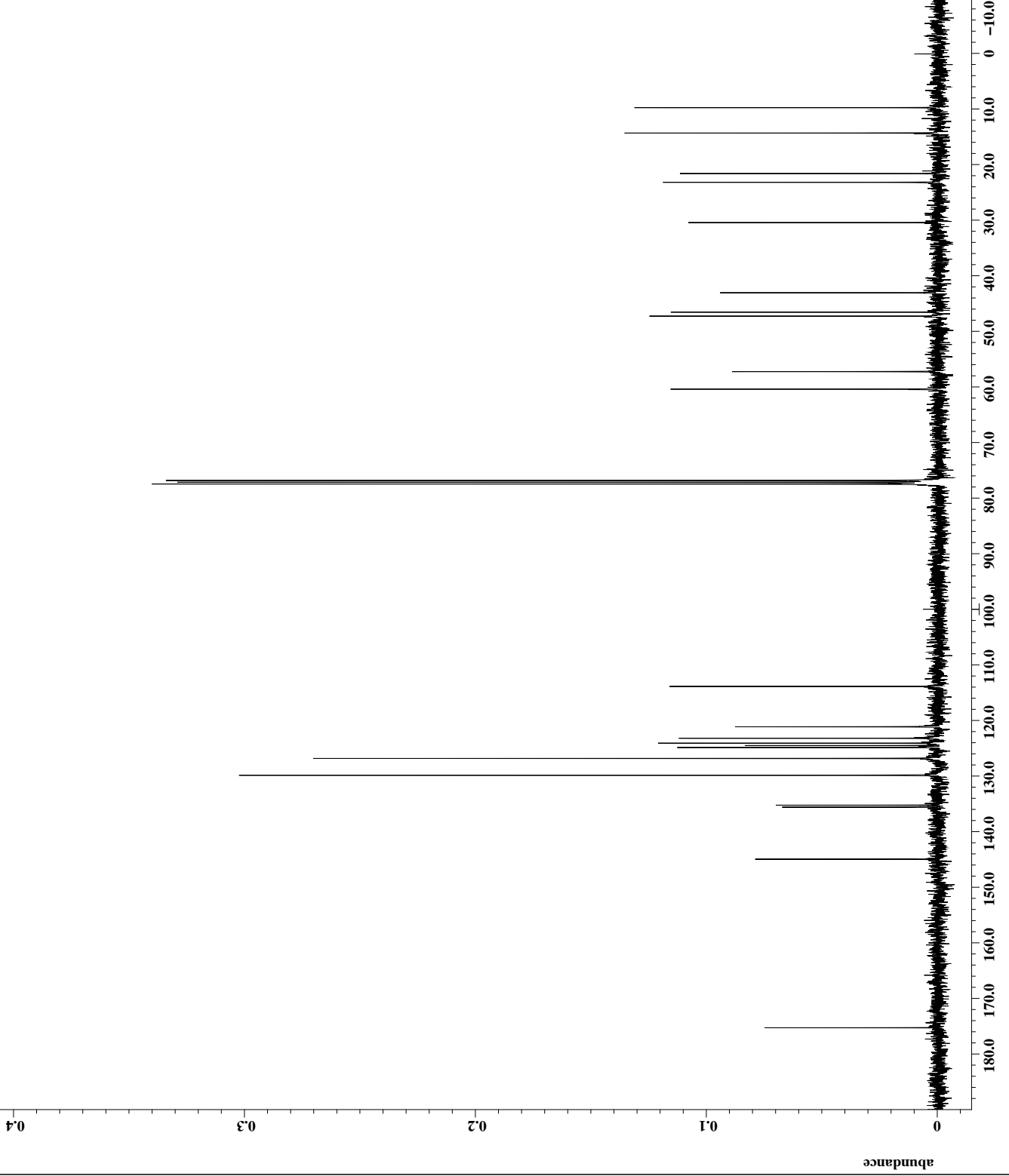
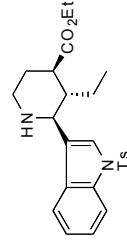
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.2[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 2.8[dB]
X_pulse = 5.6[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get = 15.5[dC]

```



Filename = 13C_NH-1.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#497764
Solvent = CHLOROFORM-D
Creation_time = 13-FEB-2008 13:59:29
Revision_time = 13-FEB-2008 14:02:29
Current_time = 25-AUG-2010 17:27:52
Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 95
Total_scans = 95
X_90_width = 9.6[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 7.8[db]
X_pulse = 4.8[us]
Irr_atn_dec = 21.4[db]
Irr_atn_noe = 21.4[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 22.9[dc]



```

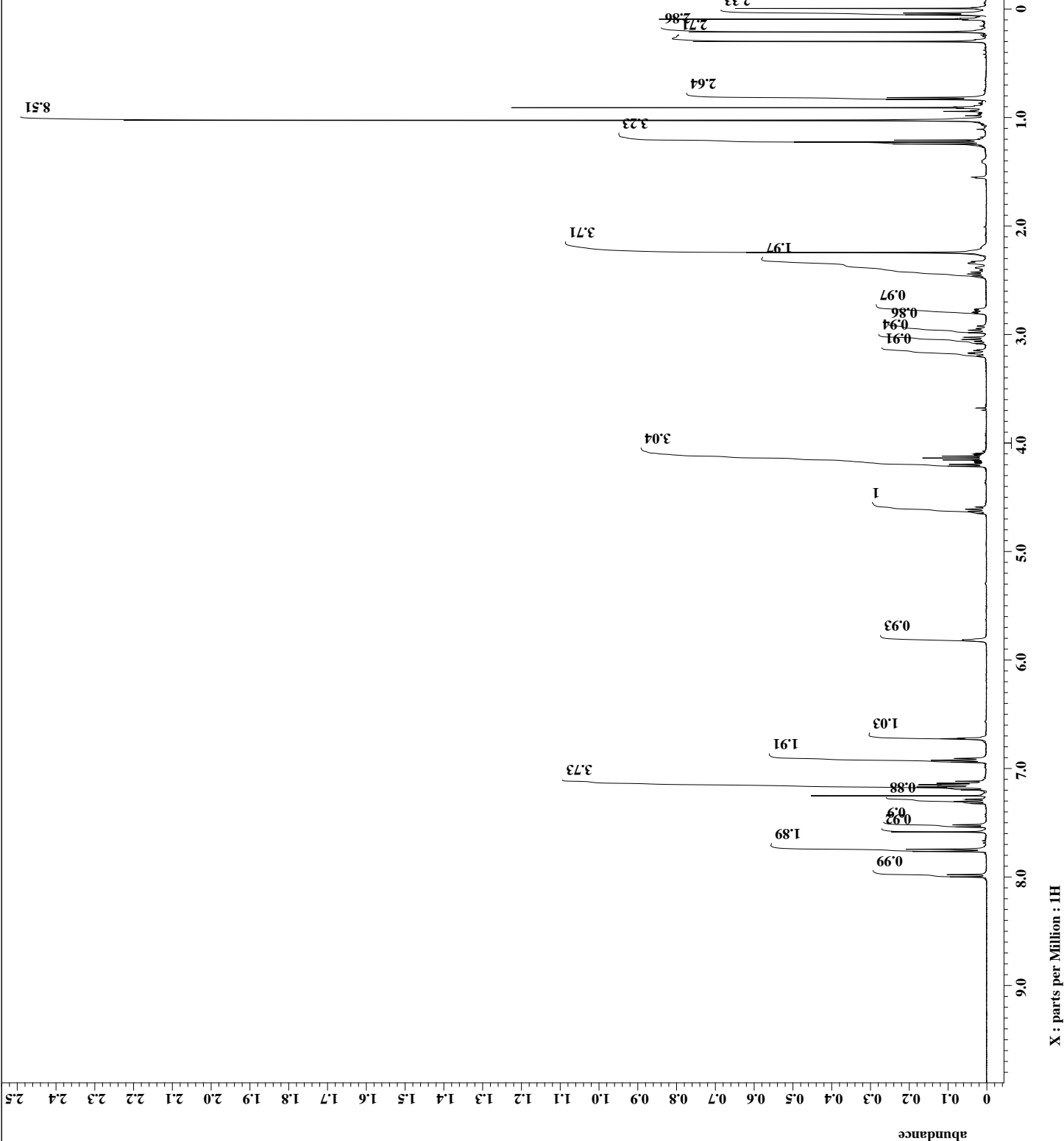
File      = 1H OH TBS-3.jdf
Author    = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent   = CHLOROFORM-D
Creation_time = 18-FEB-2009 09:09:18
Revision_time = 24-AUG-2010 19:13:57
Current_time = 24-AUG-2010 19:14:43

Comment   = single_pulse
Data_format = ID COMPLEX
Dim_size  = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site      = ECX400M
Spectrometer = DELTA2_NMR

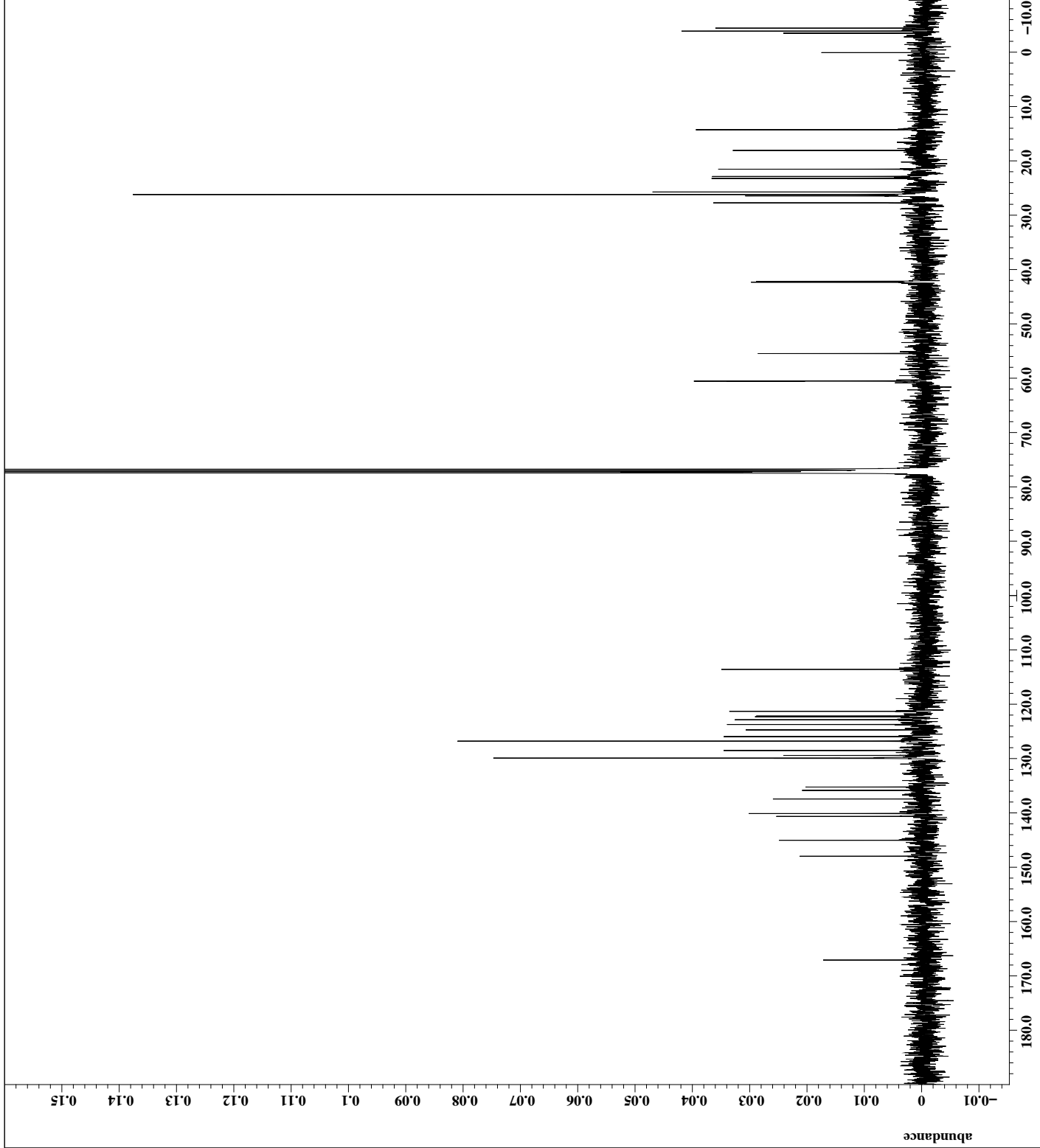
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain       = 1H
X_freq         = 399.78219838[MHz]
X_offset       = 4[ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.22897343[Hz]
X_sweep        = 7.5030012[KHz]
Irr_domain     = 1H
Irr_freq       = 399.78219838[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 399.78219838[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width     = 10.5[us]
X_acq_time     = 4.36731904[s]
X_angle        = 45[deg]
X_atn          = 1.4[dB]
X_pulse        = 5.25[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 34
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get       = 24[dc]

```



X : parts per Million : 1H



```

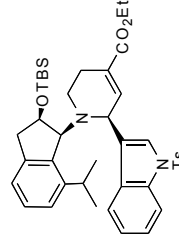
Filename = 13C OH TBS-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 18-FEB-2009 10:01:23
Revision_time = 24-AUG-2010 19:14:53
Current_time = 24-AUG-2010 19:15:47

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 369
Total_scans = 369

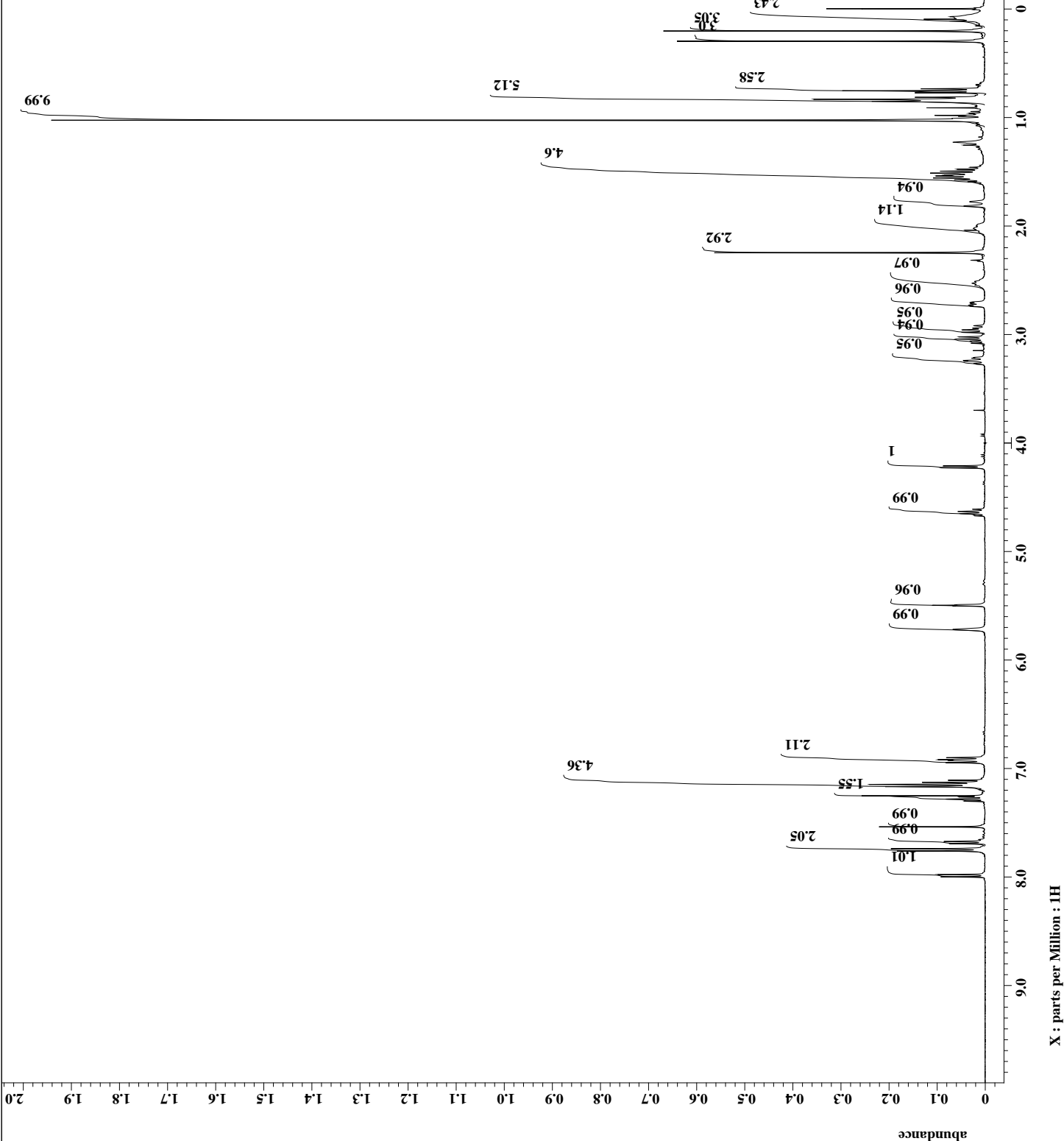
X_90_width = 8.4[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.2[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 54
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.5[dc]

```



23

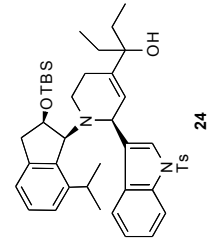
X : parts per Million : 13C



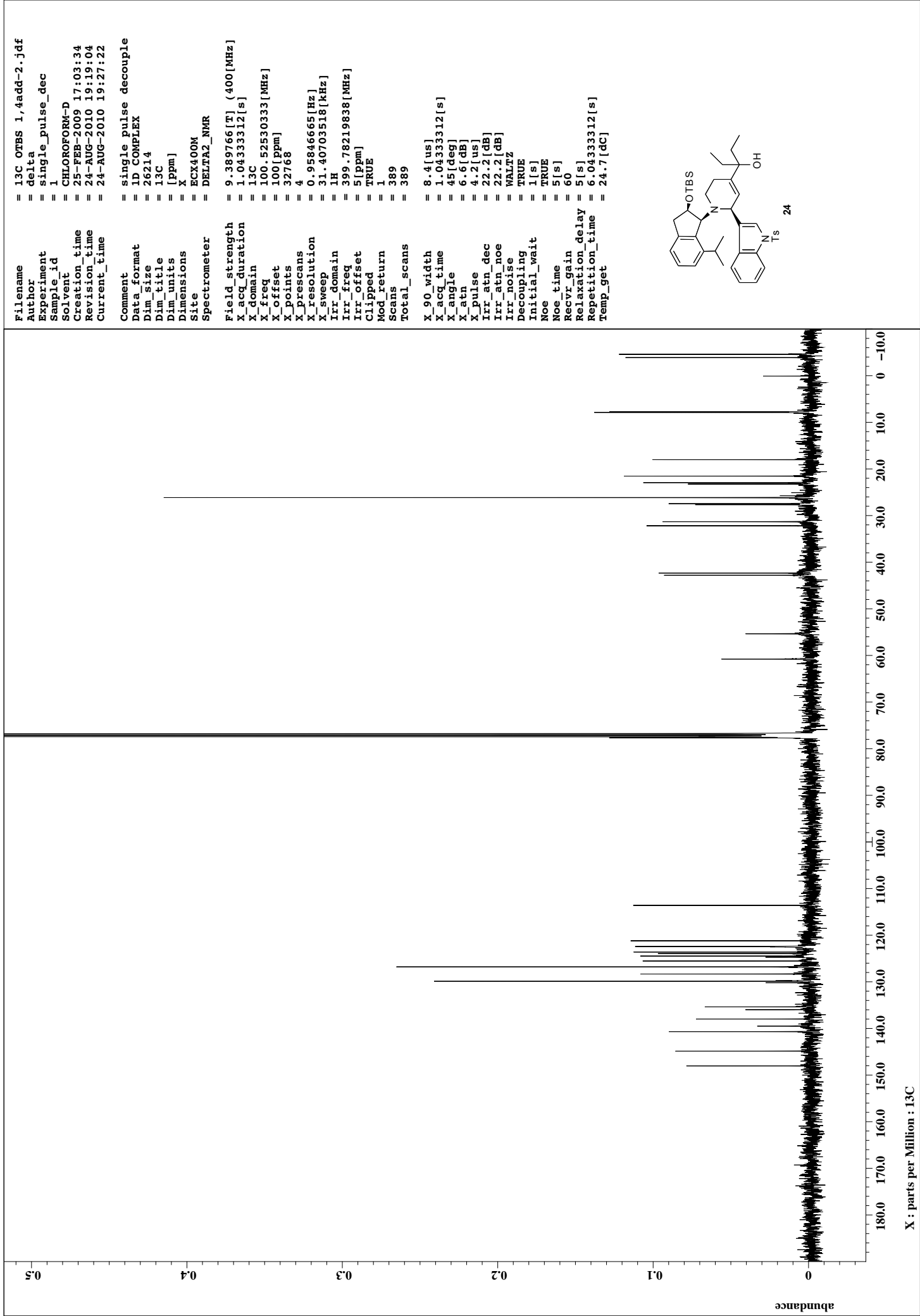
Filename = 1H_OTBS_1_4add-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 1
 Solvent = CHLOROFORM-D
 Creation_time = 25-FEB-2009 14:20:33
 Revision_time = 24-AUG-2010 19:17:39
 Current_time = 24-AUG-2010 19:18:34
 Comment = single_pulse
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR

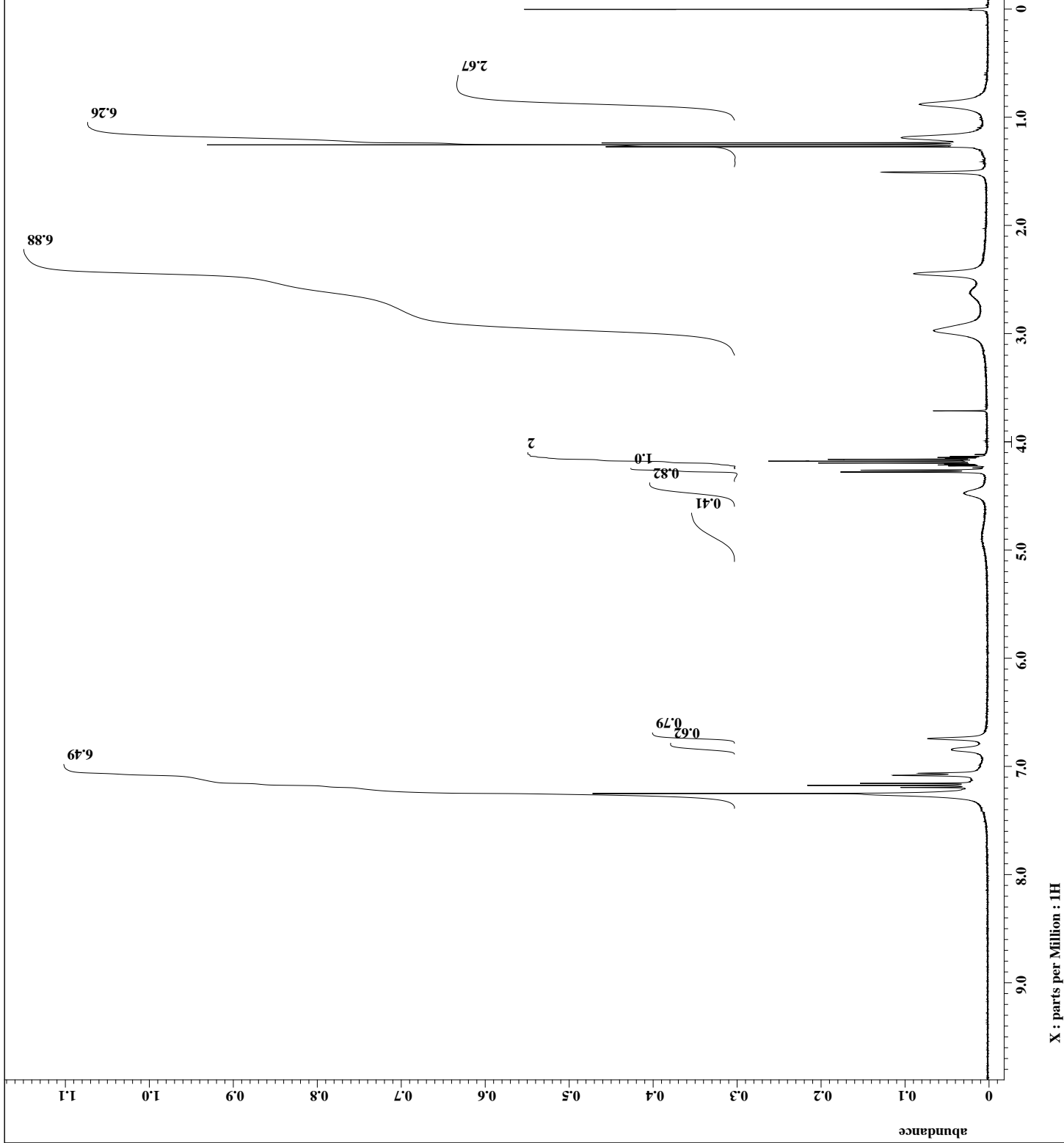
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 4[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[KHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 10.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 1.4[dB]
 X_pulse = 5.25[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 1[s]
 Repetition_time = 5.36731904[s]
 Temp_get = 24.4[dC]



X : parts per Million : 1H





```

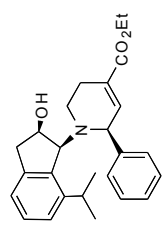
Filename = 1H Ph CO2Et OH 500C-3
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2010 16:28:13
Revision_time = 24-AUG-2010 19:30:52
Current_time = 24-AUG-2010 19:31:16

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.5[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get = 50[dc]

```



27a

X : parts per Million : 1H

```

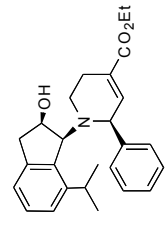
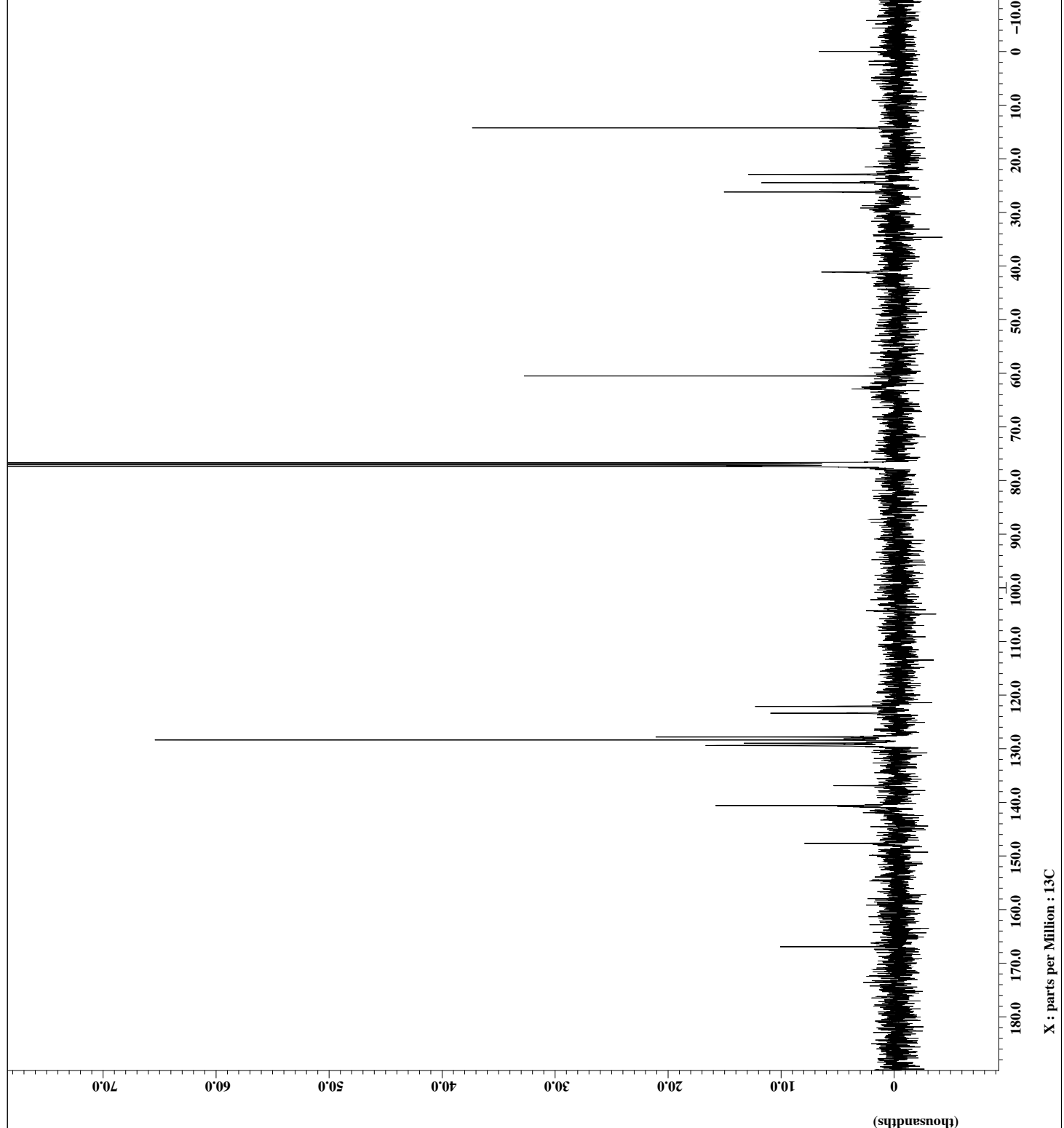
Filename = 13C Ph CO2Et OH-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#627854
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2010 17:21:43
Revision_time = 24-AUG-2010 19:31:32
Current_time = 24-AUG-2010 19:32:09

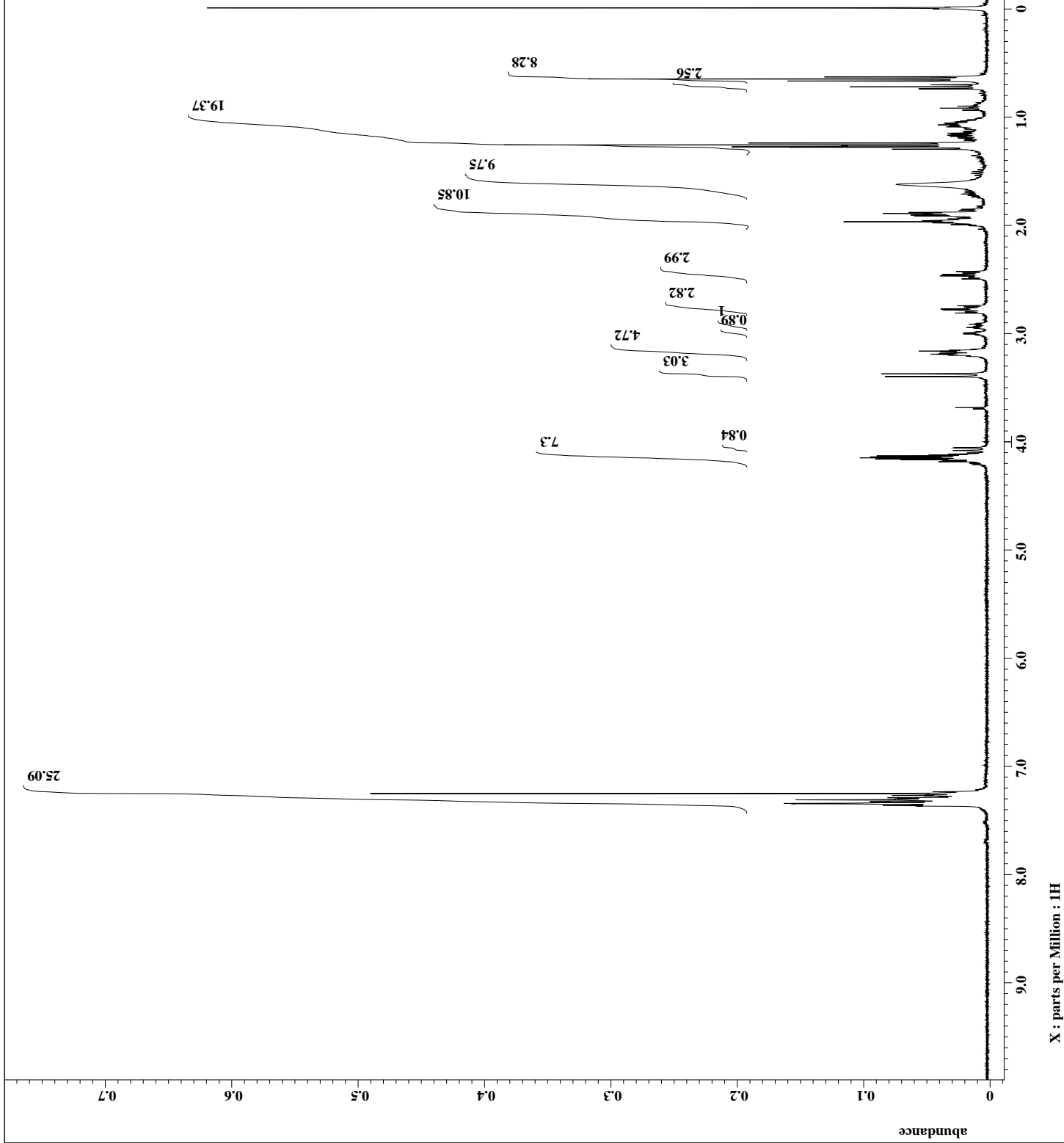
Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 501
Total_scans = 501

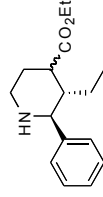
X_90_width = 9.2[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 6.6[db]
x_pulse = 4.6[us]
Irr_atn_dec = 22.2[db]
Irr_atn_noe = 22.2[db]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 50[dc]

```





Filename = 1H NH Ph Et CO2Et-3.j
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 1
 Solvent = CHLOROFORM-D
 Creation_time = 8-FEB-2010 18:51:37
 Revision_time = 24-AUG-2010 20:15:54
 Current_time = 24-AUG-2010 20:16:32
 Comment = single_pulse
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 4[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[KHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8
 X_90_width = 10.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 1.4[dB]
 X_pulse = 5.25[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 38
 Relaxation_delay = 1[s]
 Repetition_time = 5.36731904[s]
 Temp_get = 24.7[dC]



29a 1:2.7

X : parts per Million : 1H

```

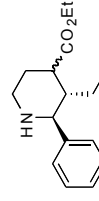
Filename = 13C NH Ph Et CO2Et-2.
Author = delta
Experiment = single_pulse_dec
Sample_id = S#503006
Solvent = CHLOROFORM-D
Creation_time = 27-FEB-2010 13:20:05
Revision_time = 24-AUG-2010 20:16:47
Current_time = 24-AUG-2010 20:18:53

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

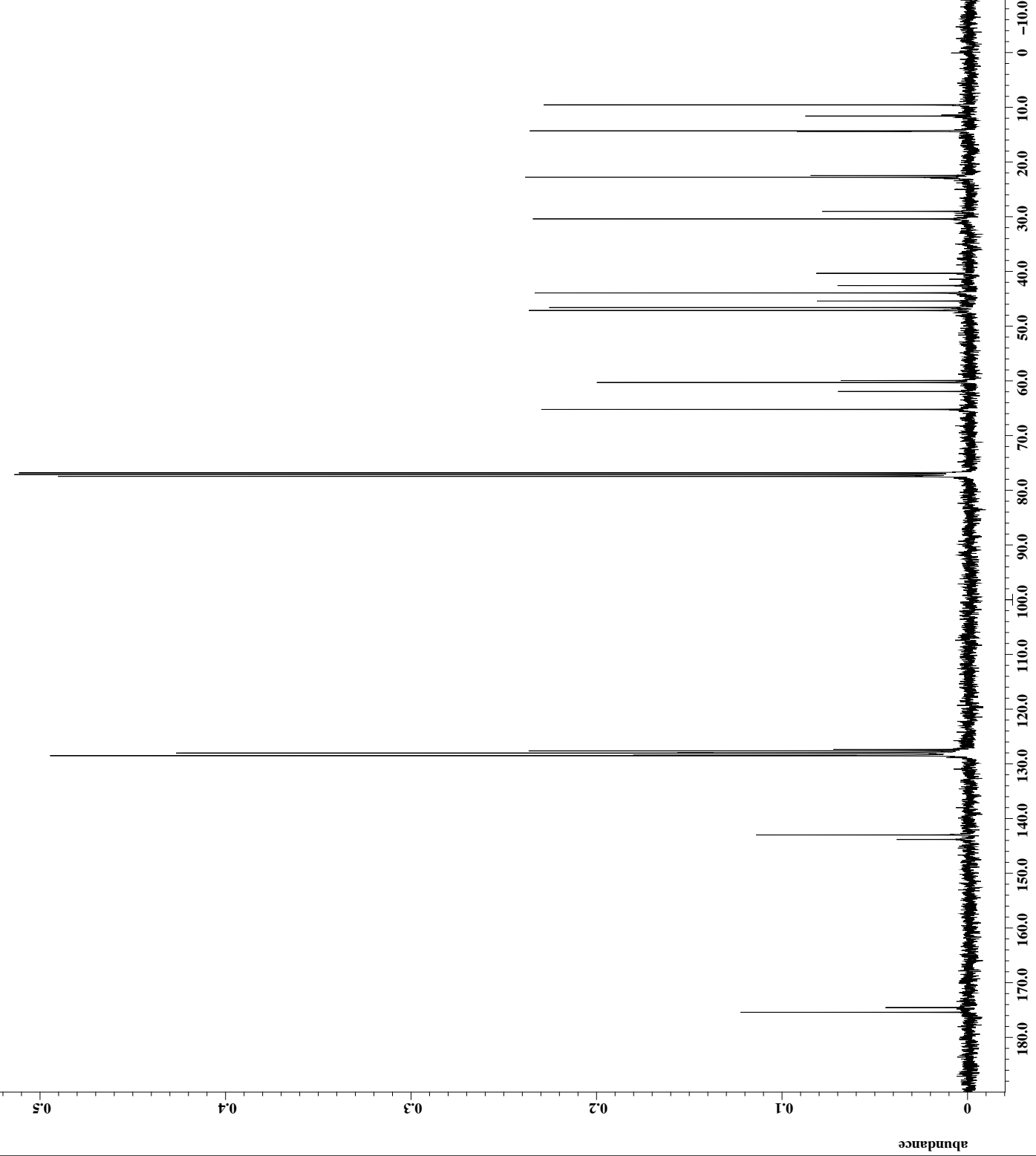
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 172
Total_scans = 172

X_90_width = 9.2[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 6.6[db]
x_pulse = 4.6[us]
Irr_atn_dec = 22.2[db]
Irr_atn_noe = 22.2[db]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 54
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.9[dc]

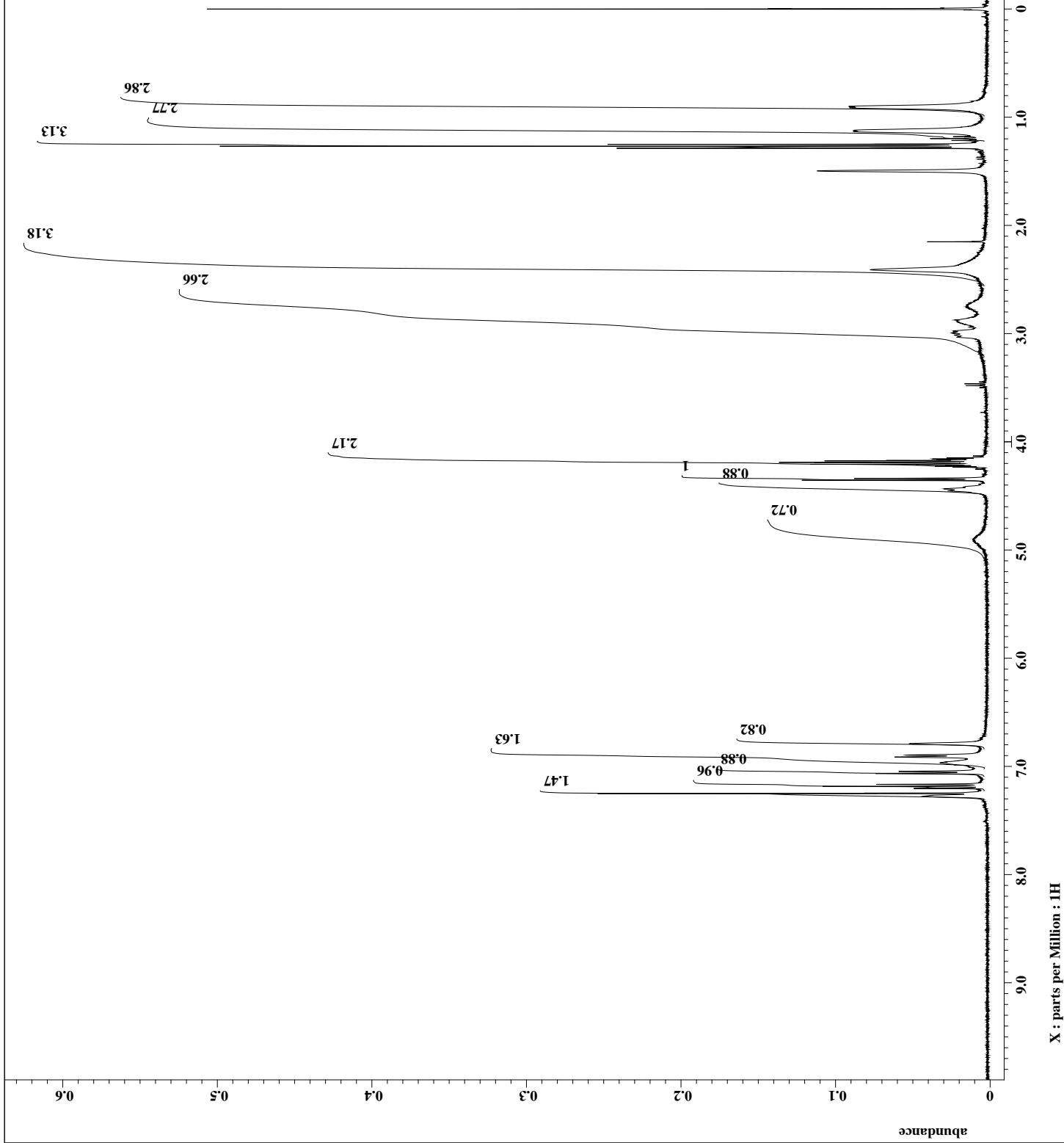
```



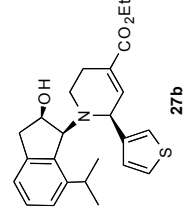
29a 1 : 2.7



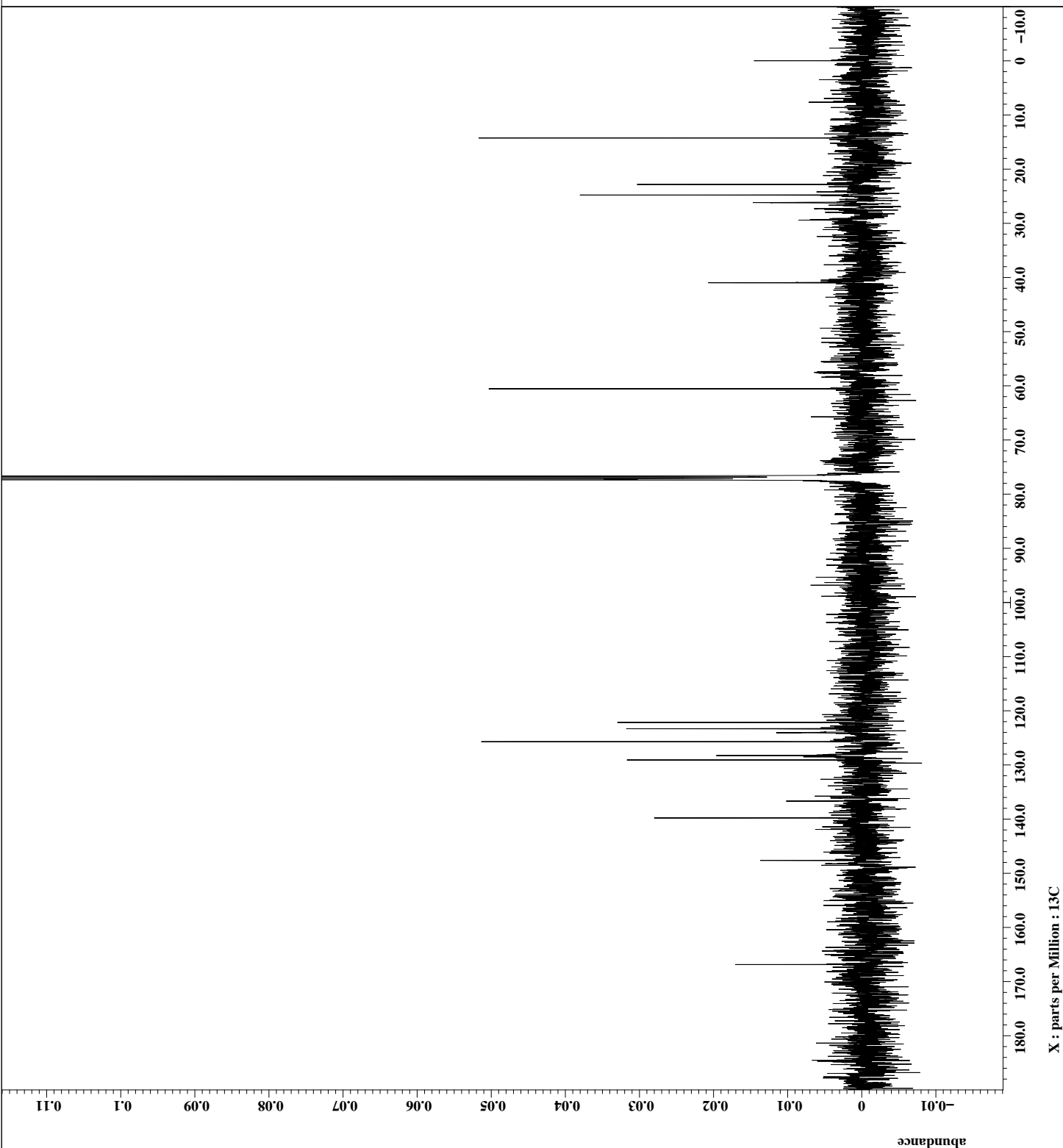
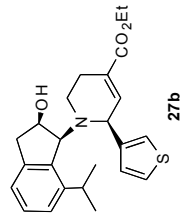
X : parts per Million : 13C



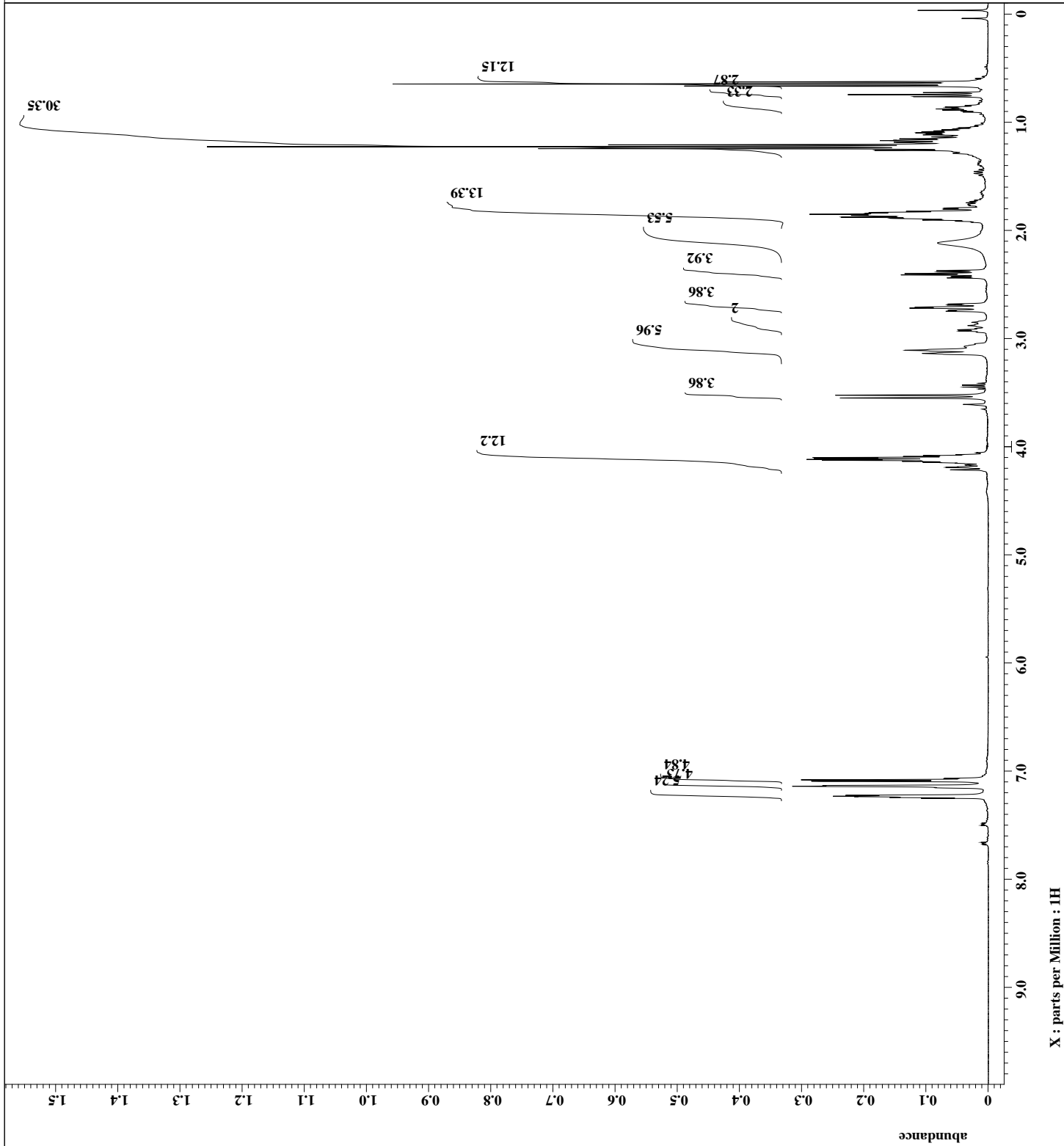
Filename = 1H thiophene CO2Et OH
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 1
 Solvent = CHLOROFORM-D
 Creation_time = 17-AUG-2010 12:34:34
 Revision_time = 24-AUG-2010 20:49:51
 Current_time = 24-AUG-2010 20:50:18
 Comment = single_pulse
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 4[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[KHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8
 X_90_width = 10.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 1.4[dB]
 X_pulse = 5.25[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 36
 Relaxation_delay = 1[s]
 Repetition_time = 5.36731904[s]
 Temp_get = 50[dc]



Filename = 13C thiophene CO2Et 0
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#487921
 Solvent = CHLOROFORM-D
 Creation_time = 17-AUG-2010 13:29:44
 Revision_time = 24-AUG-2010 20:47:32
 Current_time = 24-AUG-2010 20:48:04
 Comment = single pulse decouple
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 506.0
 Total_scans = 506.0
 X_90_width = 9.2[us]
 X_acq_time = 1.04333312[s]
 X_angle = 45[deg]
 X_atn = 6.6[db]
 X_pulse = 4.6[us]
 Irr_atn_dec = 22.2[db]
 Irr_atn_noe = 22.2[db]
 Irr_noise = WAITZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 5[s]
 Recvr_gain = 58
 Relaxation_delay = 5[s]
 Repetition_time = 6.04333312[s]
 Temp_get = 50[dc]



X : parts per Million : 13C

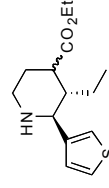


Filename = 1H NH thiophene Et CO
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 1
 Solvent = CHLOROFORM-D
 Creation_time = 17-AUG-2010 13:58:36
 Revision_time = 24-AUG-2010 20:54:47
 Current_time = 24-AUG-2010 20:55:03
 Comment = single_pulse
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 4[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[KHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8
 X_90_width = 10.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 1.4[dB]
 X_pulse = 5.25[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 26
 Relaxation_delay = 1[s]
 Repetition_time = 5.36731904[s]
 Temp_get = 25.1[dC]

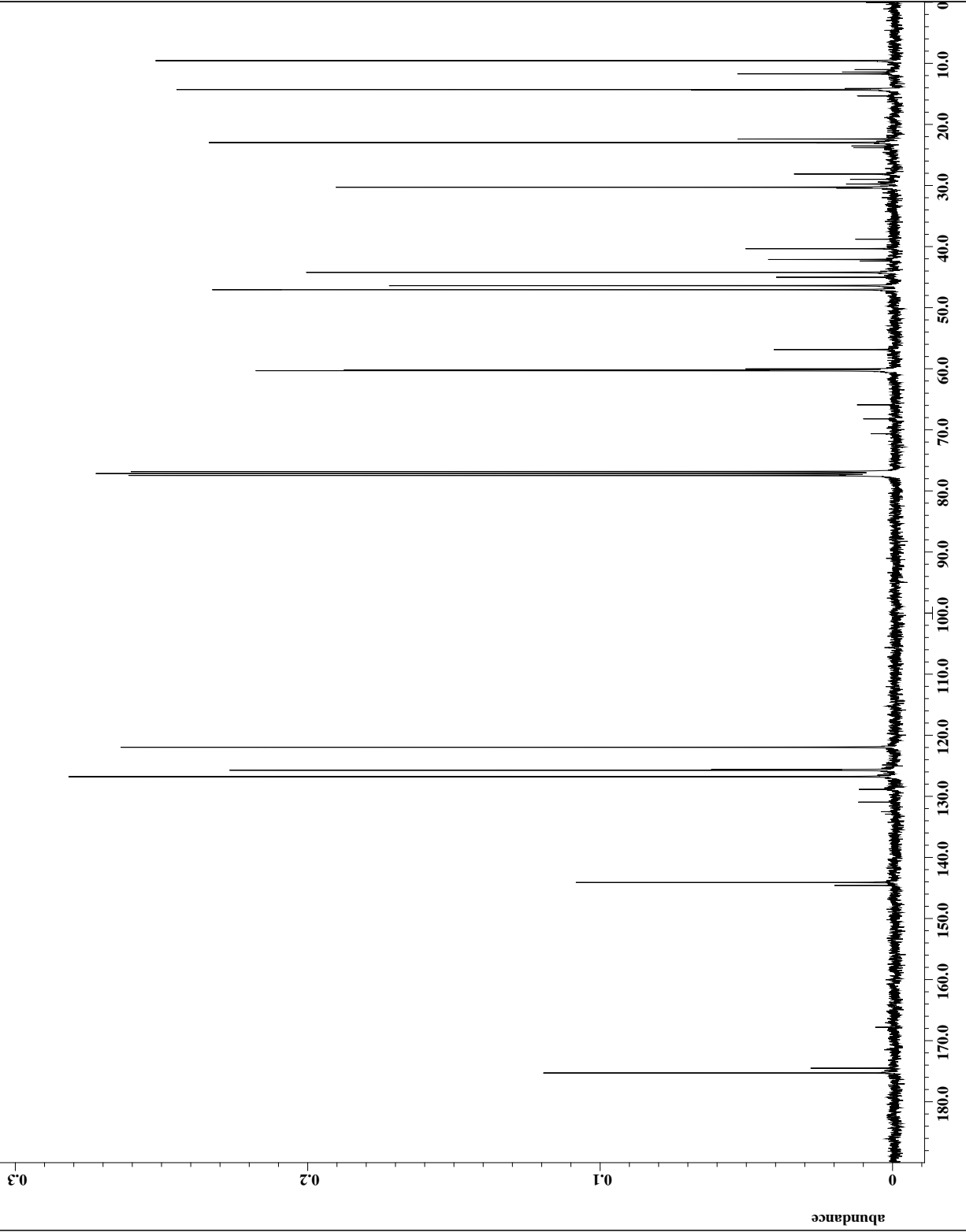
29b 1:3.8

X : parts per Million : 1H

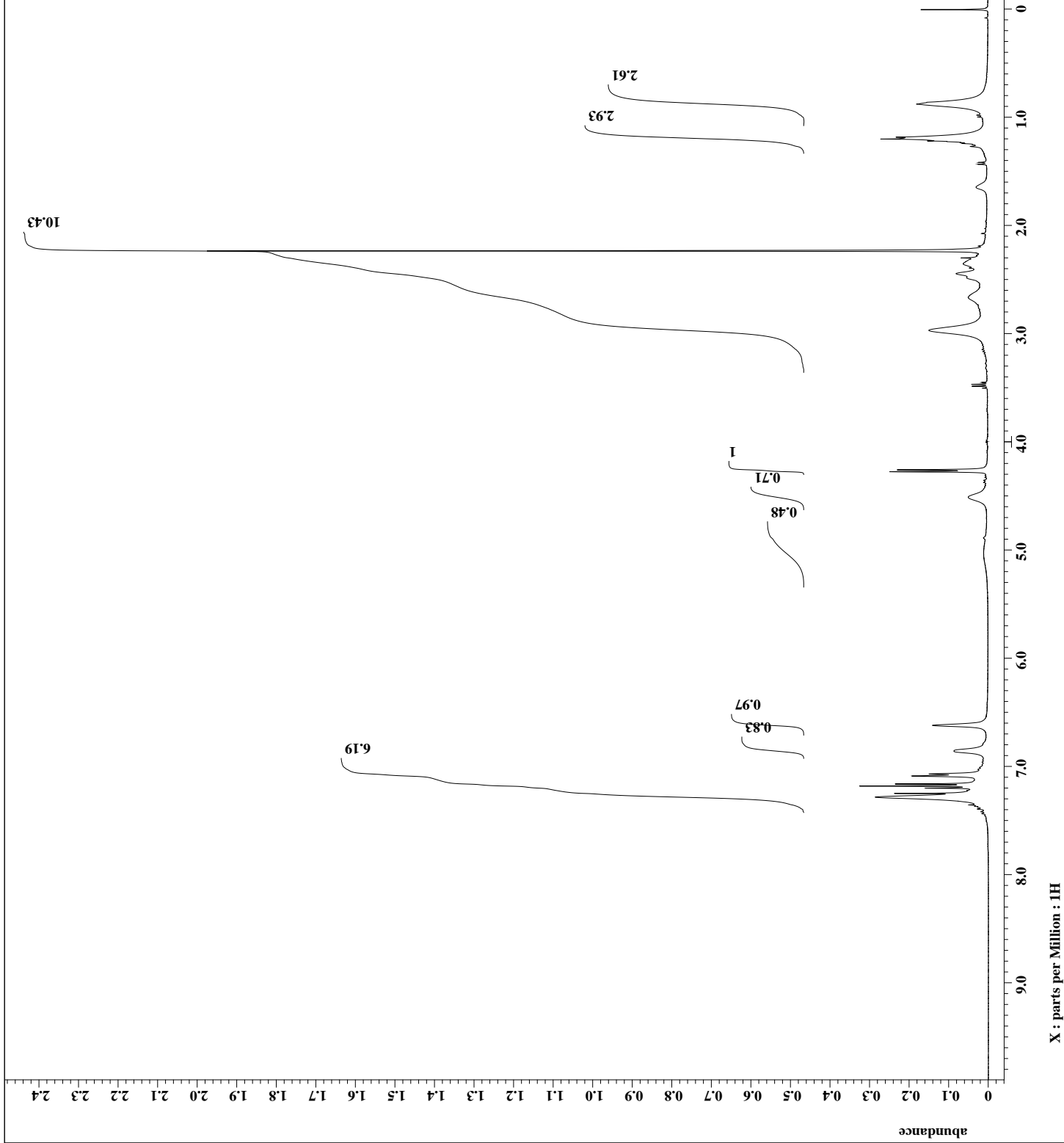
Filename = 13C NH thiophene Et C
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#538183
 Solvent = CHLOROFORM-D
 Creation_time = 17-AUG-2010 14:32:18
 Revision_time = 24-AUG-2010 20:55:44
 Current_time = 24-AUG-2010 20:56:09
 Comment = single pulse decouple
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 x_acq_duration = 1.04333312[s]
 x_domain = 13C
 x_freq = 100.52530333[MHz]
 x_offset = 100[ppm]
 x_points = 32768
 x_prescans = 4
 x_resolution = 0.95846665[Hz]
 x_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 298
 Total_scans = 298
 X_90_width = 9.2[us]
 X_acq_time = 1.04333312[s]
 X_angle = 45[deg]
 X_atn = 6.6[db]
 X_pulse = 4.6[us]
 Irr_atn_dec = 22.2[db]
 Irr_atn_noe = 22.2[db]
 Irr_noise = WAITZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 5[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 6.04333312[s]
 Temp_get = 25.1[dc]



29b 1 : 3.8



X : parts per Million : 13C



```

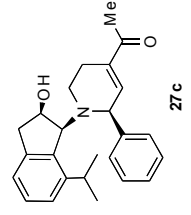
Filename = 1H Ph ketone OH 500c-
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2010 15:00:31
Revision_time = 24-AUG-2010 20:34:11
Current_time = 24-AUG-2010 20:34:52

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.5[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get = 50[dc]

```



```

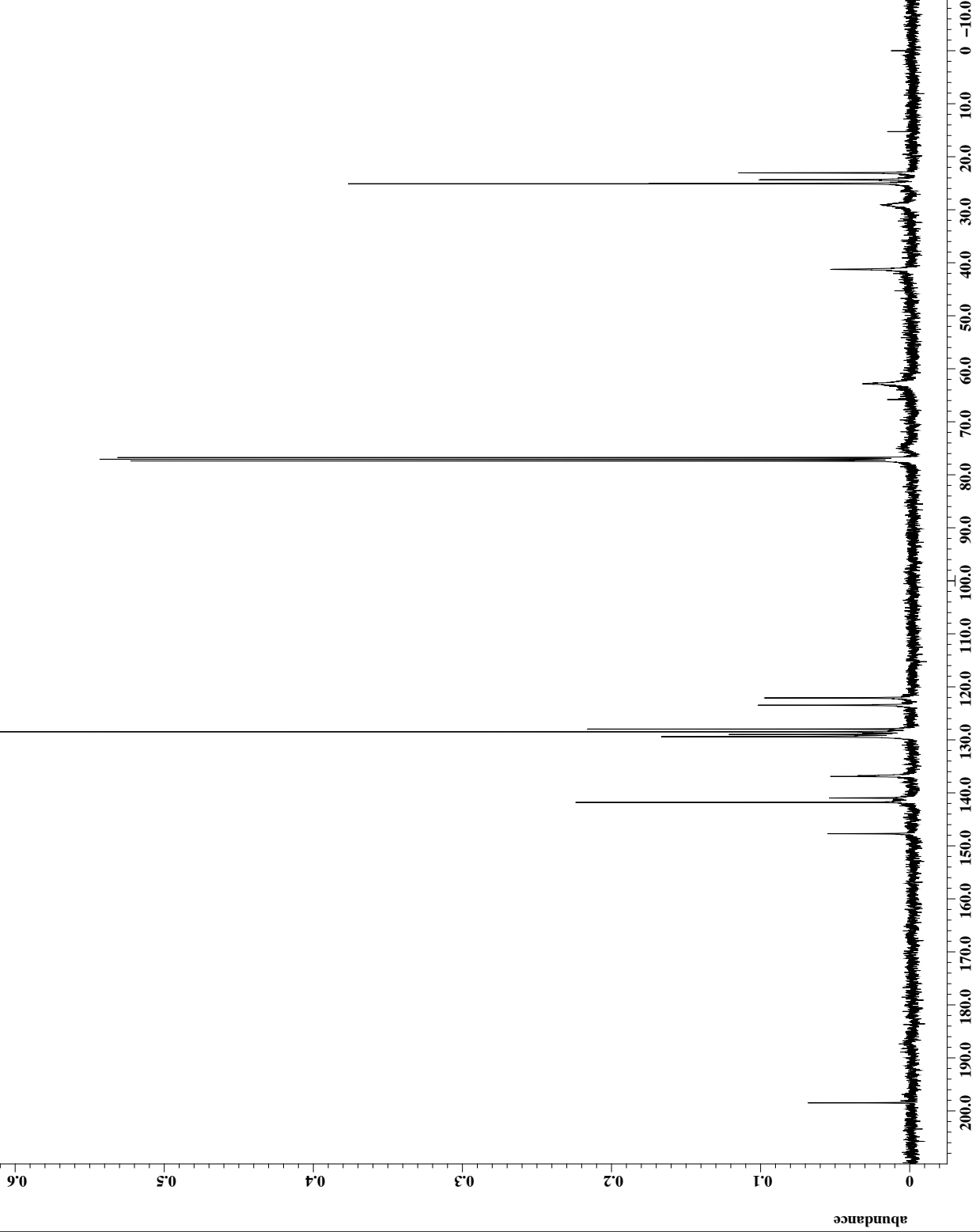
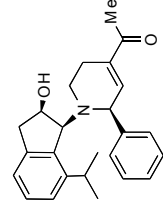
Filename = 13C Ph ketone OH-2.jd
Author = delta
Experiment = single_pulse_dec
Sample_id = S#575323
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2010 15:48:50
Revision_time = 24-AUG-2010 20:34:58
Current_time = 24-AUG-2010 20:35:43

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

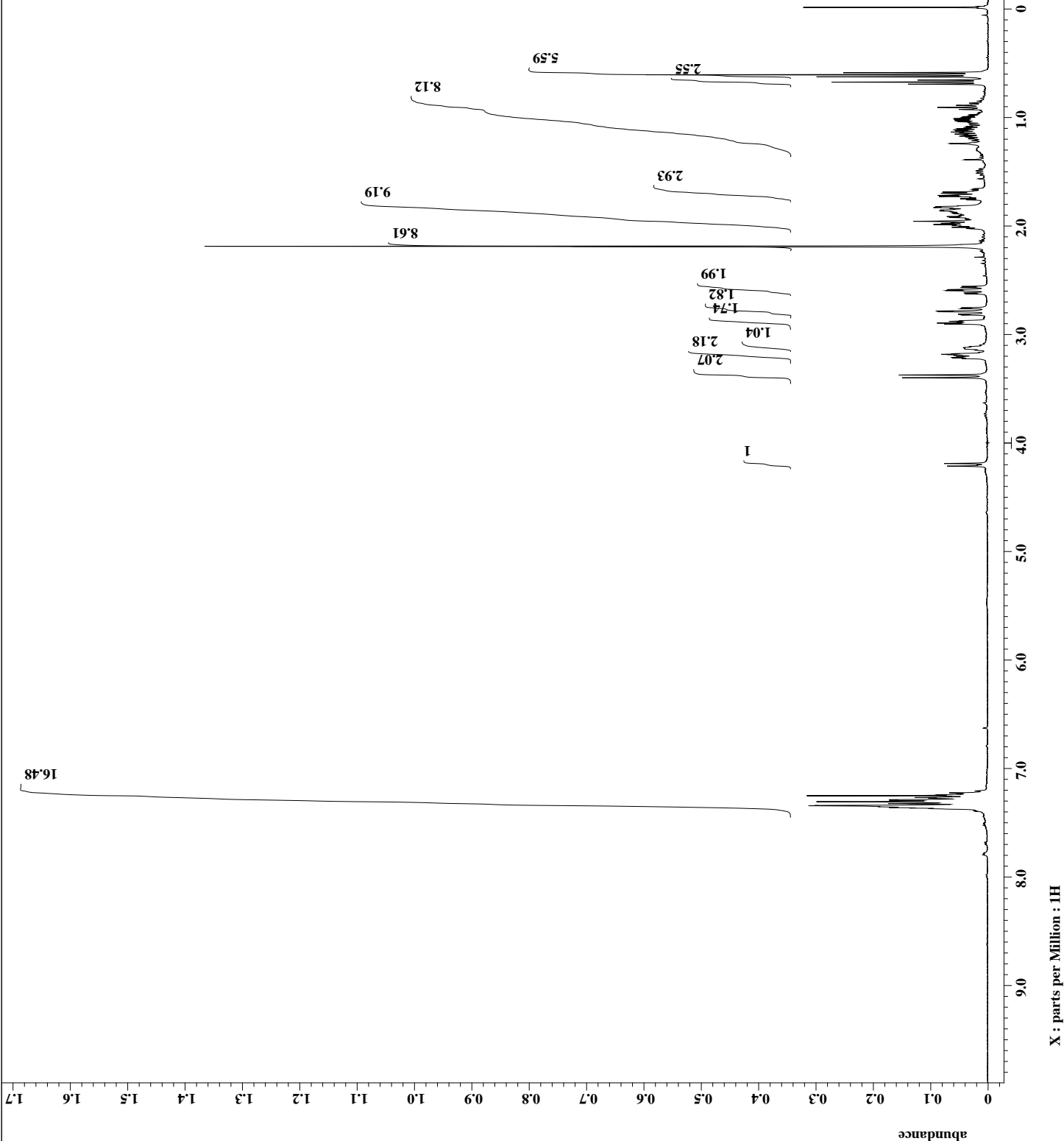
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 442
Total_scans = 442

X_90_width = 9.2[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 6.6[db]
x_pulse = 4.6[us]
Irr_atn_dec = 22.2[db]
Irr_atn_noe = 22.2[db]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 58
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 50[dc]

```



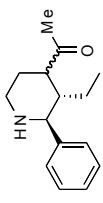
X : parts per Million : 13C



Filename = 1H NH Ph Et COME-3.jd
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 1
 Solvent = CHLOROFORM-D
 Creation_time = 15-FEB-2010 21:19:03
 Revision_time = 24-AUG-2010 20:41:55
 Current_time = 24-AUG-2010 20:42:21
 Comment = single_pulse
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 4[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[KHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 10.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 1.4[dB]
 X_pulse = 5.25[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 32
 Relaxation_delay = 1[s]
 Repetition_time = 5.36731904[s]
 Temp_get = 24.3[dc]



29c 1 : 2.2

```

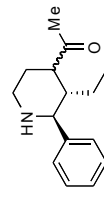
Filename = 13C NH Ph Et COME-2.j
Author = delta
Experiment = single_pulse_dec
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 27-FEB-2010 13:38:51
Revision_time = 24-AUG-2010 20:42:29
Current_time = 24-AUG-2010 20:43:02

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

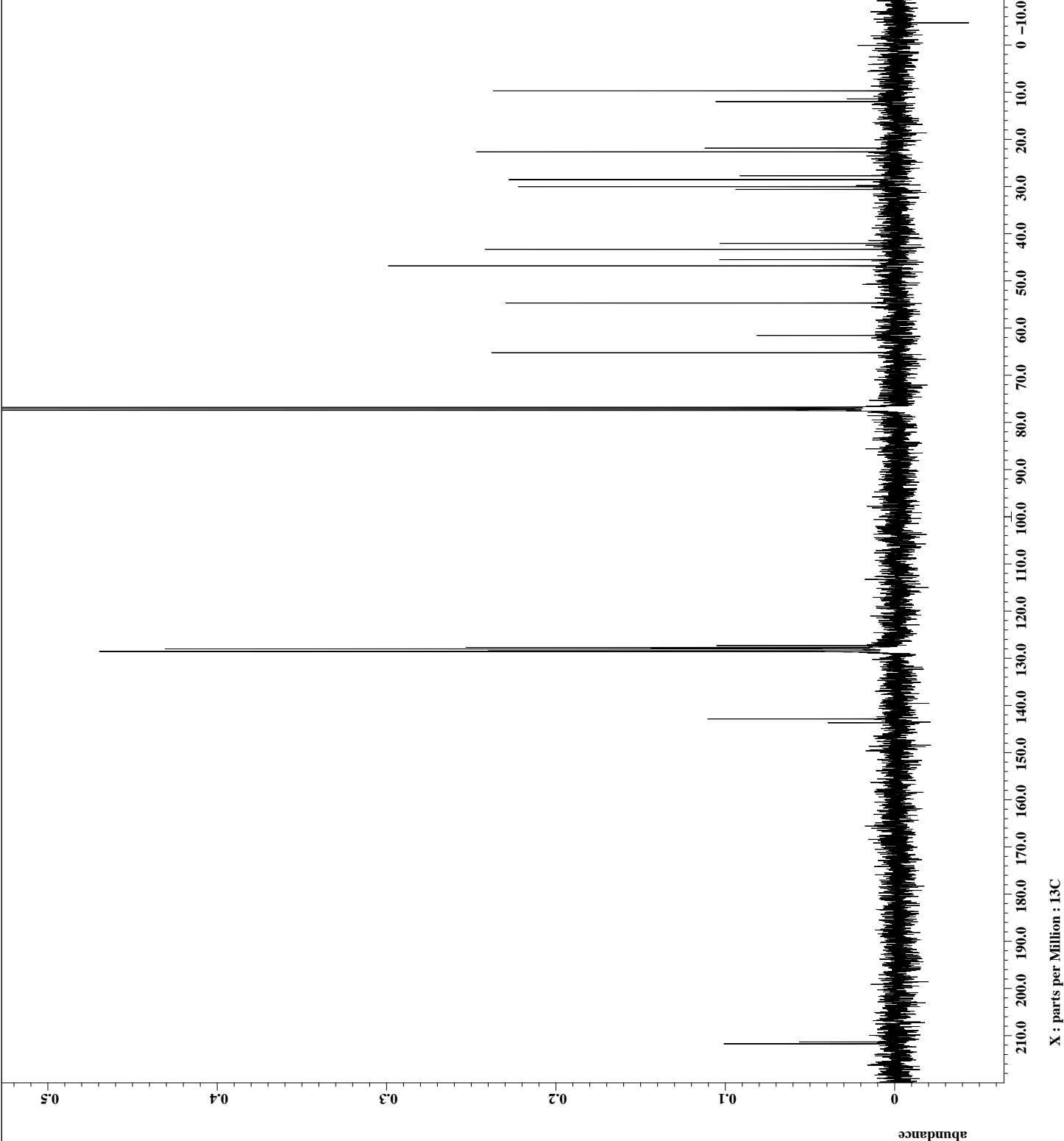
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 117
Total_scans = 117

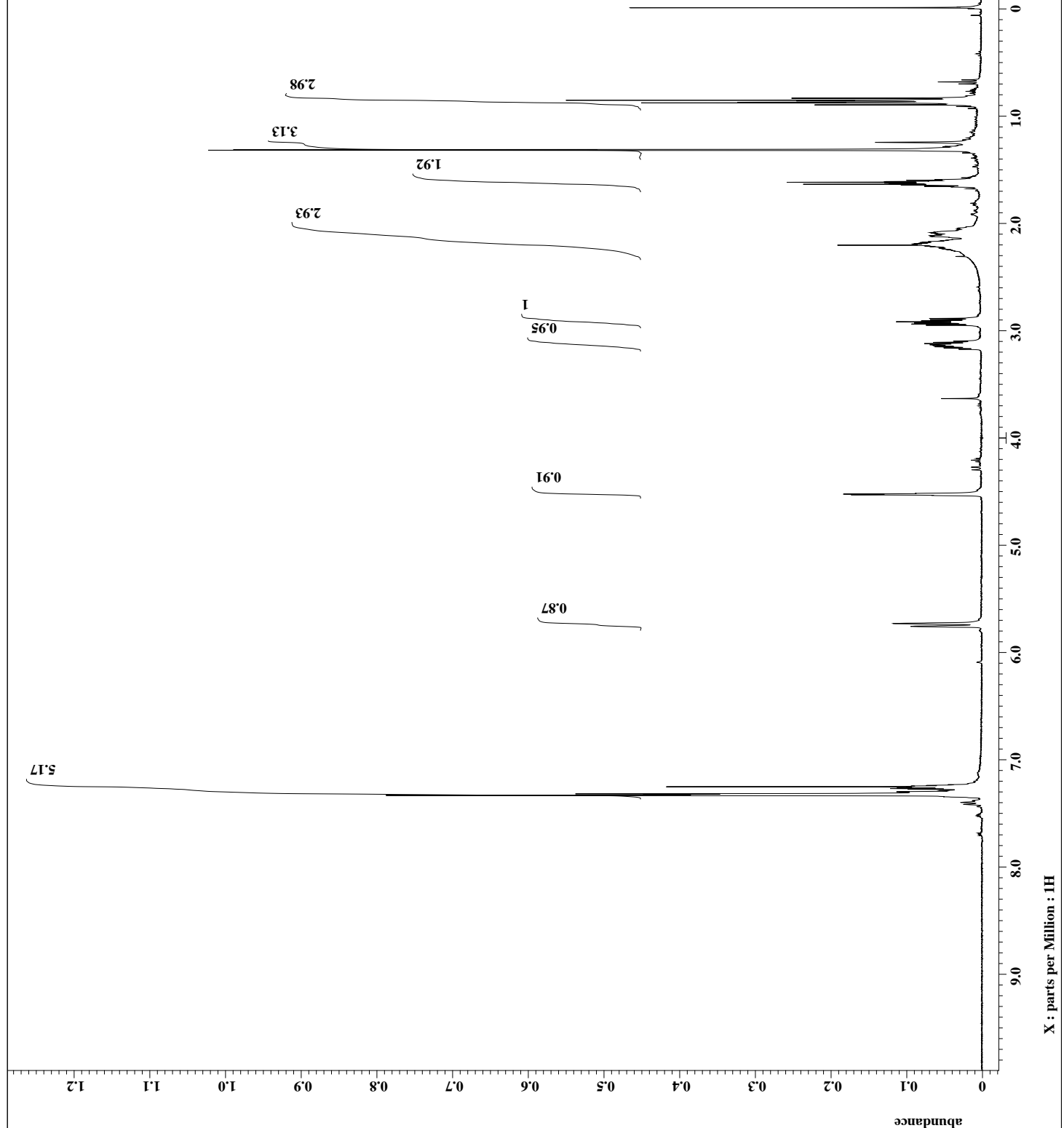
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[db]
X_pulse = 4.6[us]
Irr_atn_dec = 22.2[db]
Irr_atn_noe = 22.2[db]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 60
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 25.2[dc]

```



29c 1 : 2.2





```

Filename = 1H NH Ph CMeEtOH-3.jd
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 15-FEB-2010 21:22:09
Revision_time = 24-AUG-2010 20:46:26
Current_time = 24-AUG-2010 20:46:36

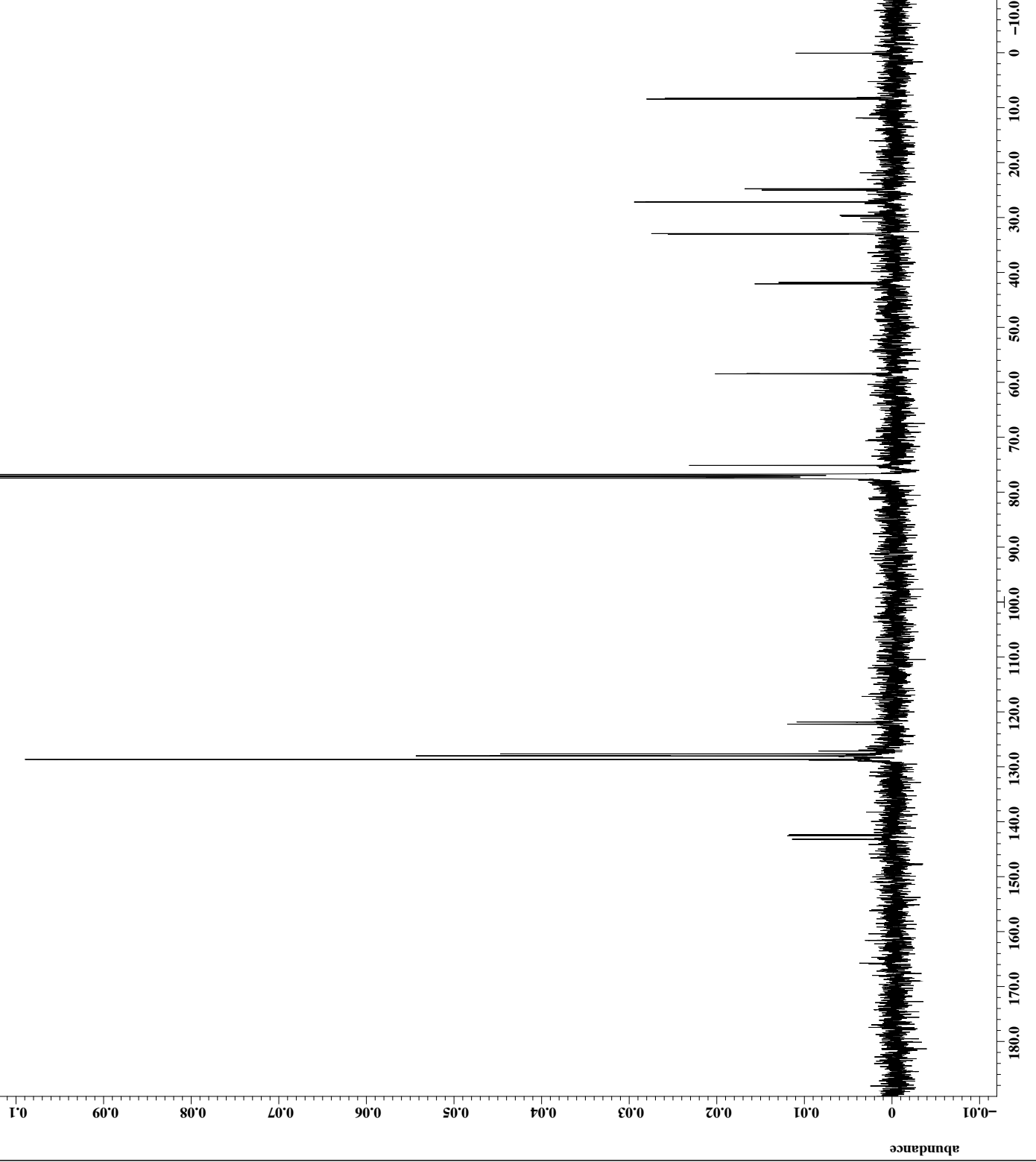
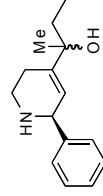
Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

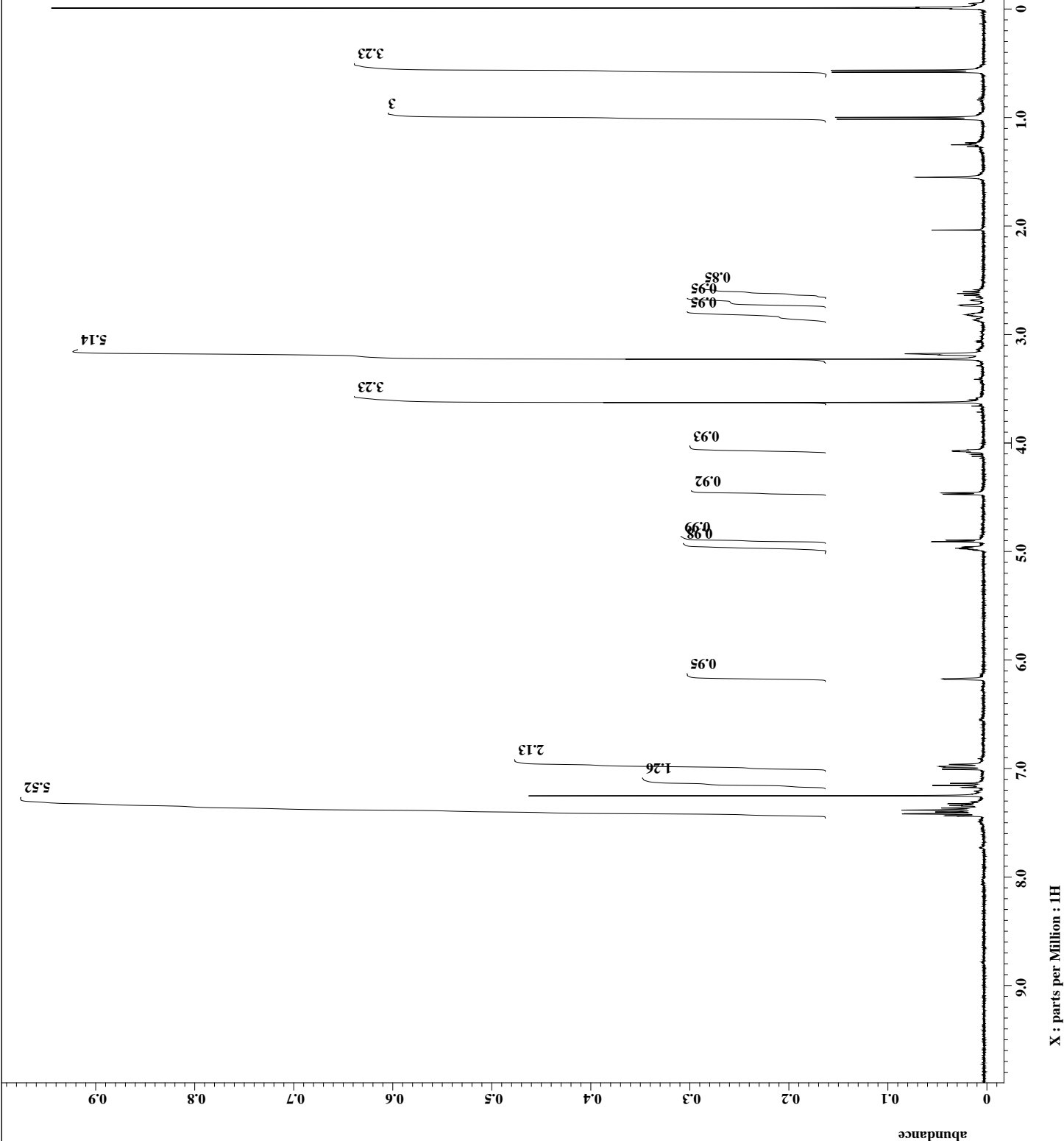
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.5[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get = 24.5[dC]

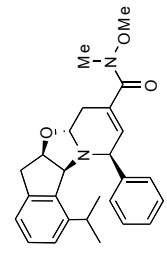
```

Filename = 13C NH Ph CMeEtOH-2.j
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#427683
 Solvent = CHLOROFORM-D
 Creation_time = 17-AUG-2010 11:50:05
 Revision_time = 24-AUG-2010 20:46:44
 Current_time = 24-AUG-2010 20:47:16
 Comment = single pulse decouple
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 514
 Total_scans = 514
 X_90_width = 9.2[us]
 X_acq_time = 1.04333312[s]
 X_angle = 45[deg]
 X_atn = 6.6[db]
 X_pulse = 4.6[us]
 Irr_atn_dec = 22.2[db]
 Irr_atn_noe = 22.2[db]
 Irr_noise = WAITZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 5[s]
 Recvr_gain = 52
 Relaxation_delay = 5[s]
 Repetition_time = 6.04333312[s]
 Temp_get = 24.6[dc]

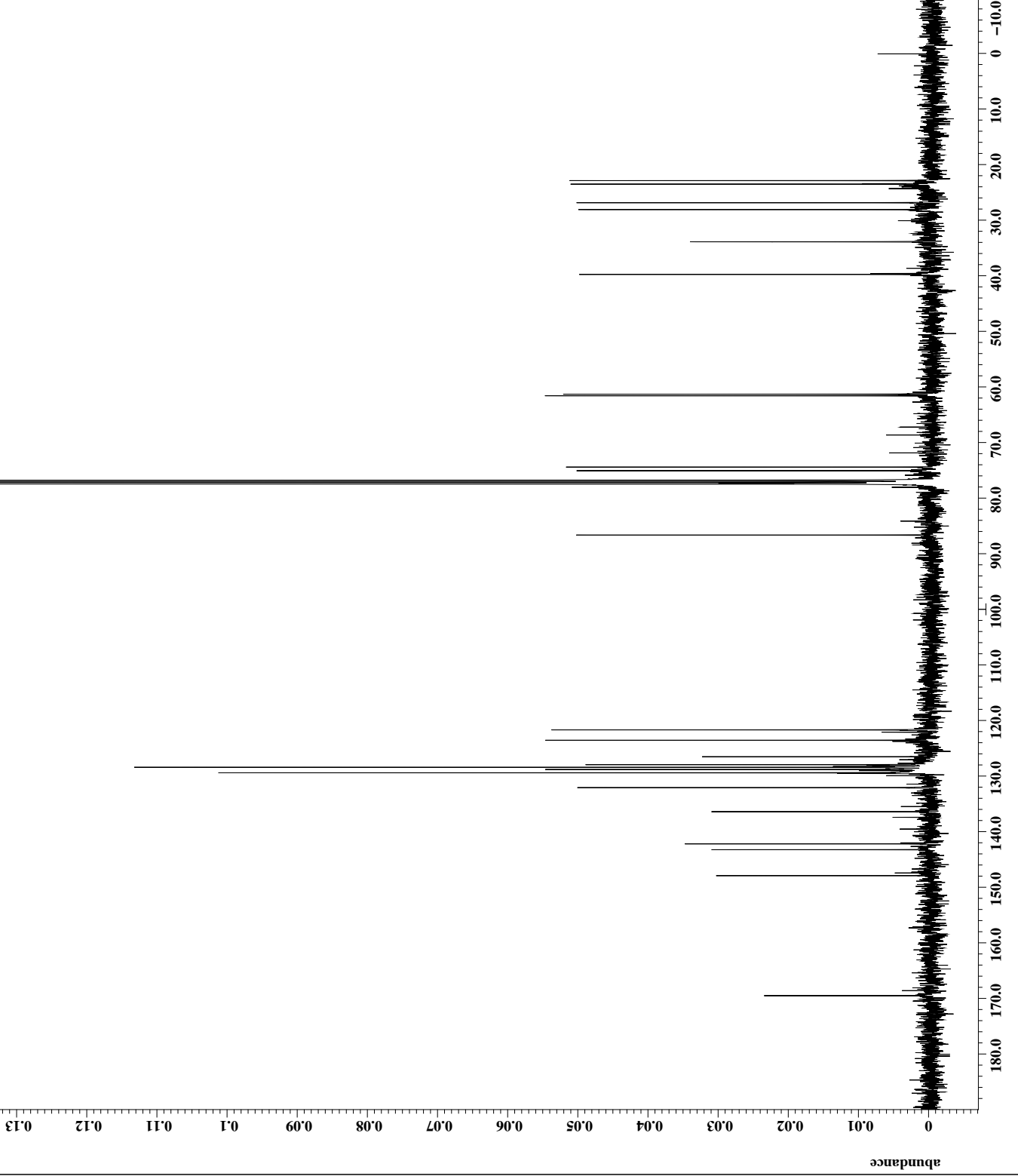
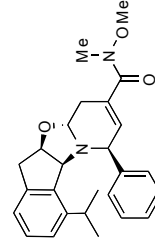


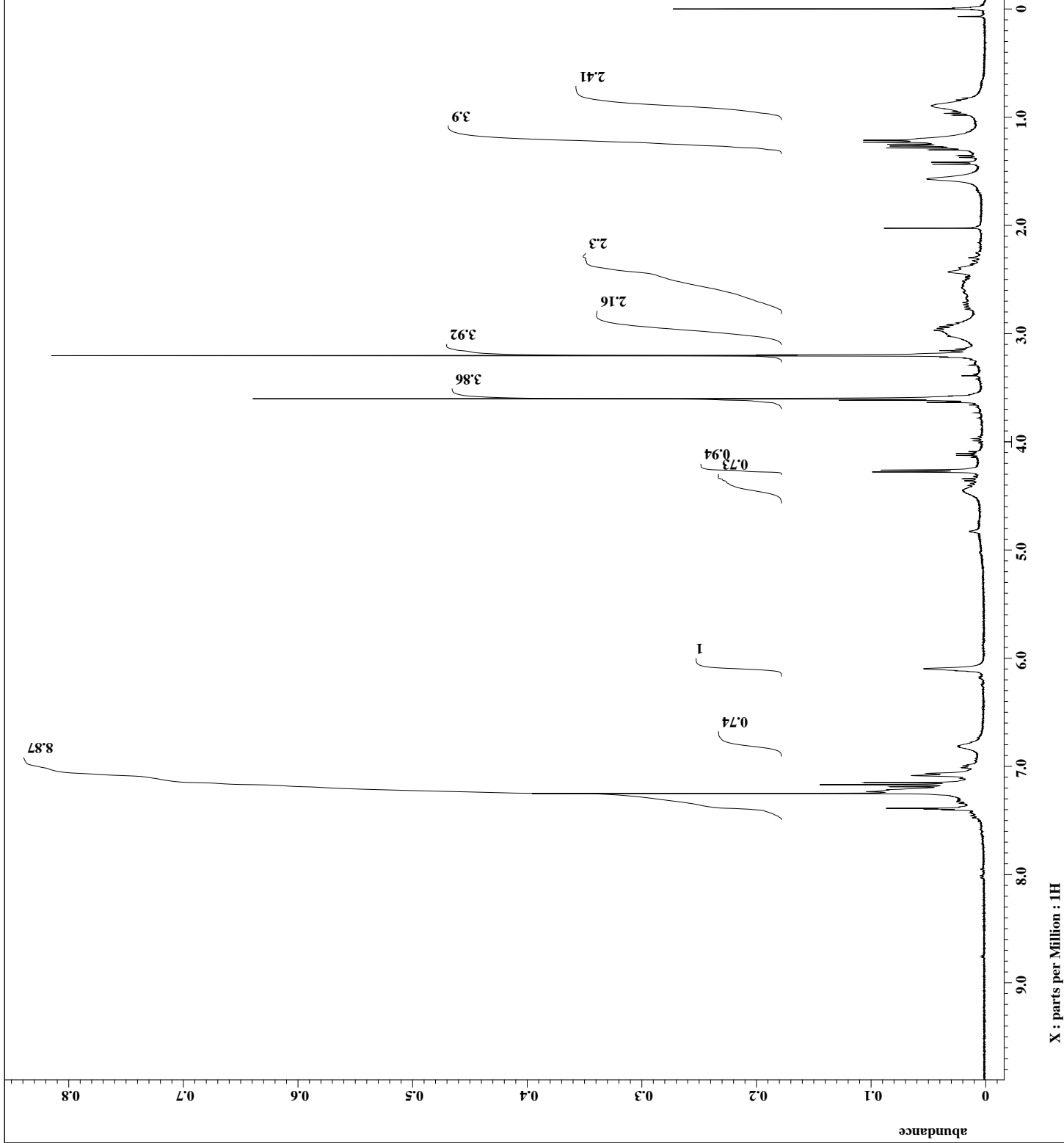


Filename = 1H OP6pAEC Ph Weinre
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 1
 Solvent = CHLOROFORM-D
 Creation_time = 12-JAN-2010 10:11:23
 Revision_time = 24-AUG-2010 20:24:12
 Current_time = 24-AUG-2010 20:24:36
 Comment = single_pulse
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 4[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[KHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8
 X_90_width = 10.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 1.4[dB]
 X_pulse = 5.25[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 1[s]
 Repetition_time = 5.36731904[s]
 Temp_get = 22.7[dc]

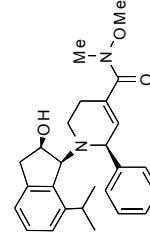


Filename = 13C OP6pAEC Ph Weinr
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#383609
 Solvent = CHLOROFORM-D
 Creation_time = 20-AUG-2010 10:18:50
 Revision_time = 24-AUG-2010 20:24:44
 Current_time = 24-AUG-2010 20:25:48
 Comment = single pulse decouple
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 423
 Total_scans = 423
 X_90_width = 9.2[us]
 X_acq_time = 1.04333312[s]
 X_angle = 45[deg]
 X_atn = 6.6[db]
 X_pulse = 4.6[us]
 Irr_atn_dec = 22.2[db]
 Irr_atn_noe = 22.2[db]
 Irr_noise = WAITZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 5[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 6.04333312[s]
 Temp_get = 25.9[dc]





Filename = 1H Ph Weinreb OH 500C
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 1
 Solvent = CHLOROFORM-D
 Creation_time = 20-AUG-2010 12:04:20
 Revision_time = 24-AUG-2010 20:31:26
 Current_time = 24-AUG-2010 20:31:39
 Comment = single_pulse
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 4[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[KHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8
 X_90_width = 10.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 1.4[dB]
 X_pulse = 5.25[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 34
 Relaxation_delay = 1[s]
 Repetition_time = 5.36731904[s]
 Temp_get = 50[dc]



```

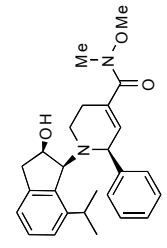
Filename = 13C Ph Weinreb 50c-6
Author = delta
Experiment = single_pulse_dec
Sample_id = S#365786
Solvent = CHLOROFORM-D
Creation_time = 26-AUG-2010 10:01:19
Revision_time = 26-AUG-2010 11:27:10
Current_time = 26-AUG-2010 11:28:04

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

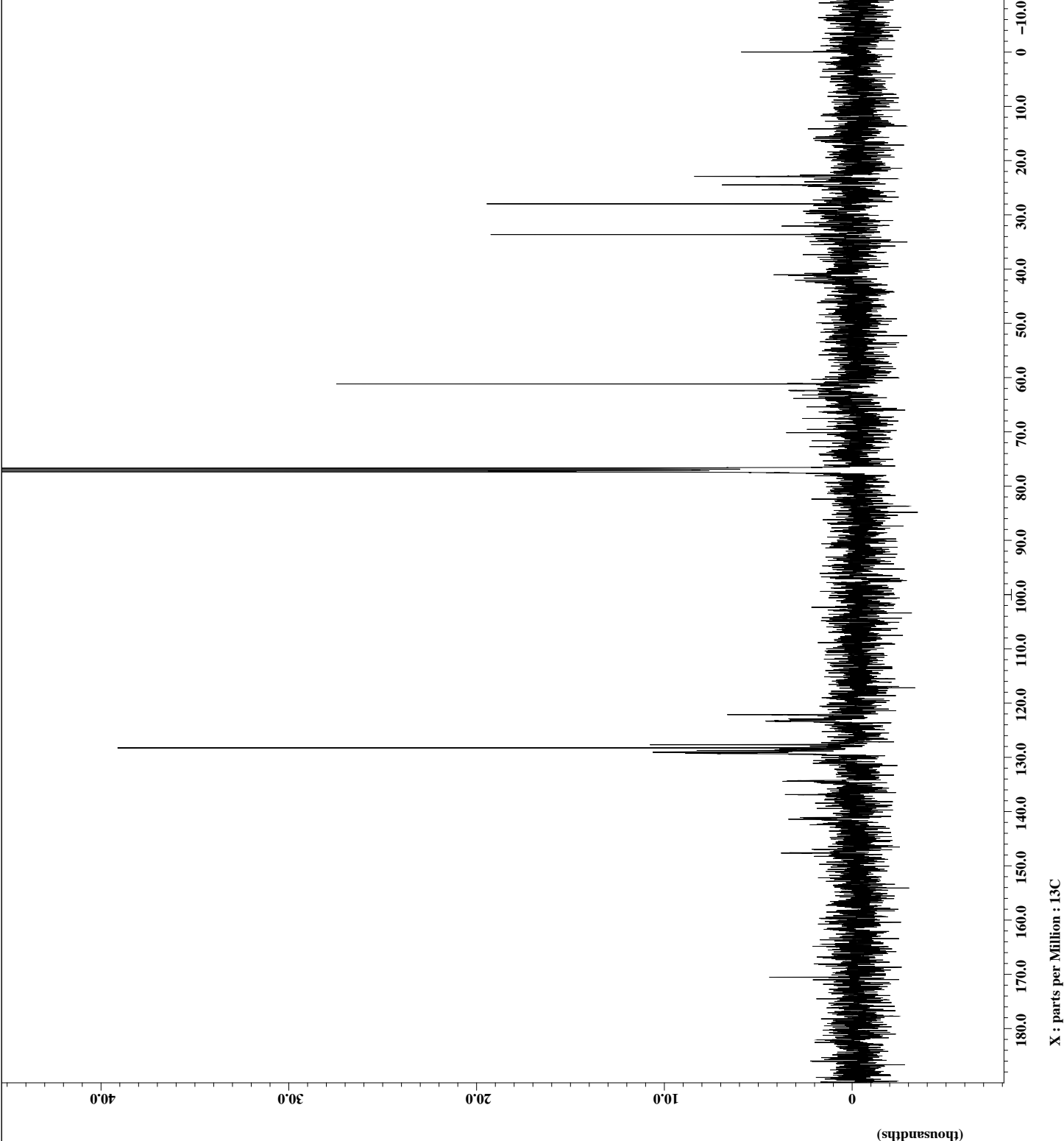
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 548
Total_scans = 548

X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[db]
X_pulse = 4.6[us]
Irr_atn_dec = 22.2[db]
Irr_atn_noe = 22.2[db]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 50[dc]

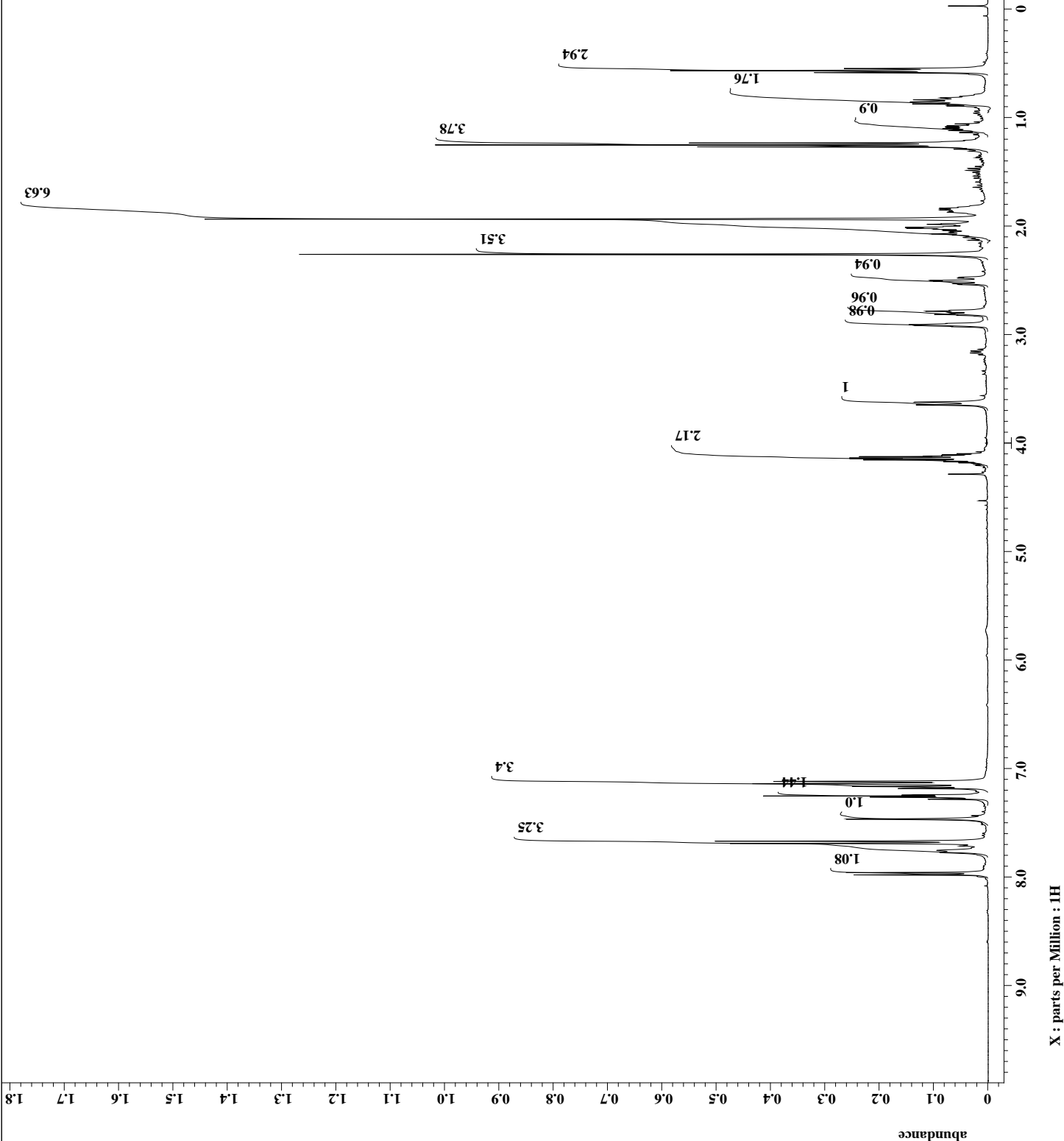
```



27d



X : parts per Million : 13C



```

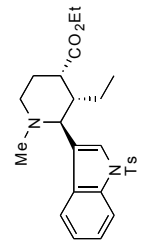
Filename = 1H N-methyl isomer-2.
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 18-FEB-2008 13:48:23
Revision_time = 24-AUG-2010 18:49:35
Current_time = 24-AUG-2010 18:51:15

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.2[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 2.8[dB]
X_pulse = 5.6[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 22
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get = 23.8[dC]

```



31a

X : parts per Million : 1H

```

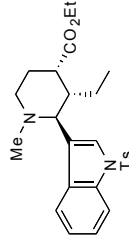
Filename = 13C N-methyl isomer-1
Author = delta
Experiment = single_pulse_dec
Sample_id = S#498967
Solvent = CHLOROFORM-D
Creation_time = 18-FEB-2008 14:02:42
Revision_time = 18-FEB-2008 14:06:07
Current_time = 24-AUG-2010 18:52:50

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

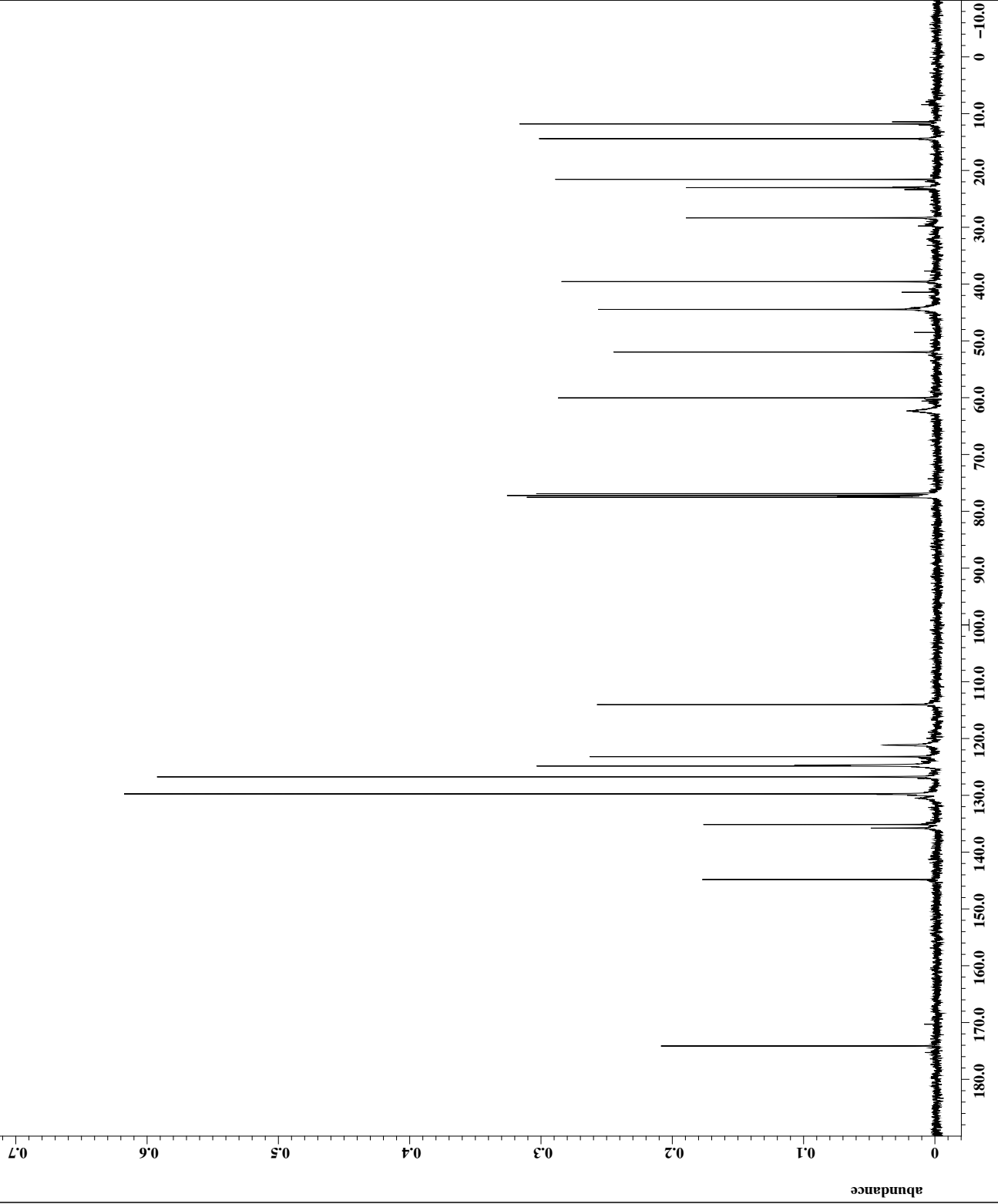
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 115.0
Total_scans = 115.0

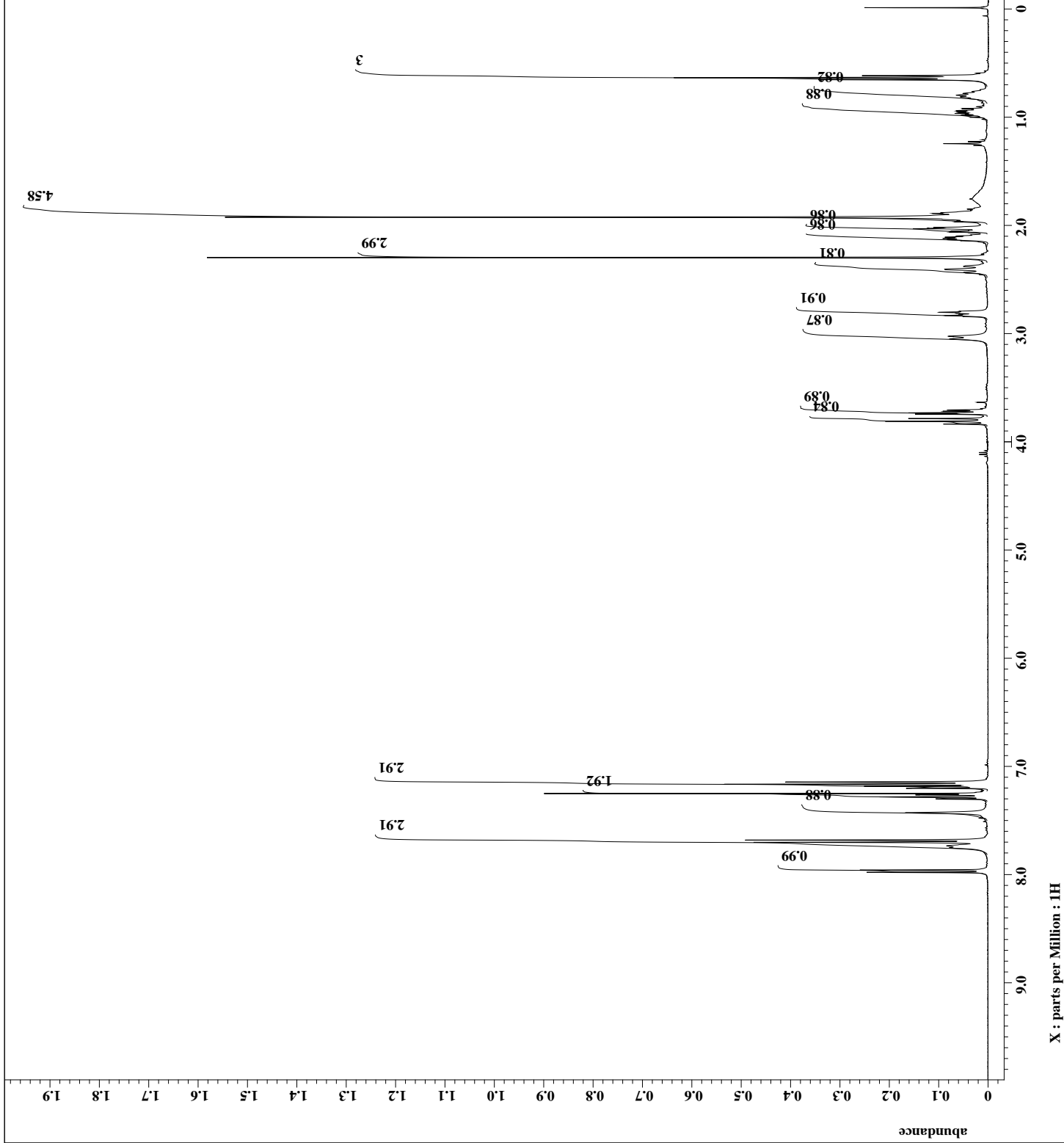
X_90_width = 9.6[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 7.8[db]
x_pulse = 4.8[us]
Irr_atn_dec = 21.4[db]
Irr_atn_noe = 21.4[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.2[dc]

```



31a





```

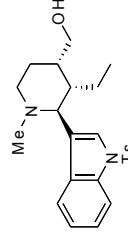
Filename = 1H alcohol isomer-3.j
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 23-APR-2010 12:41:31
Revision_time = 24-AUG-2010 18:54:38
Current_time = 24-AUG-2010 18:55:19

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

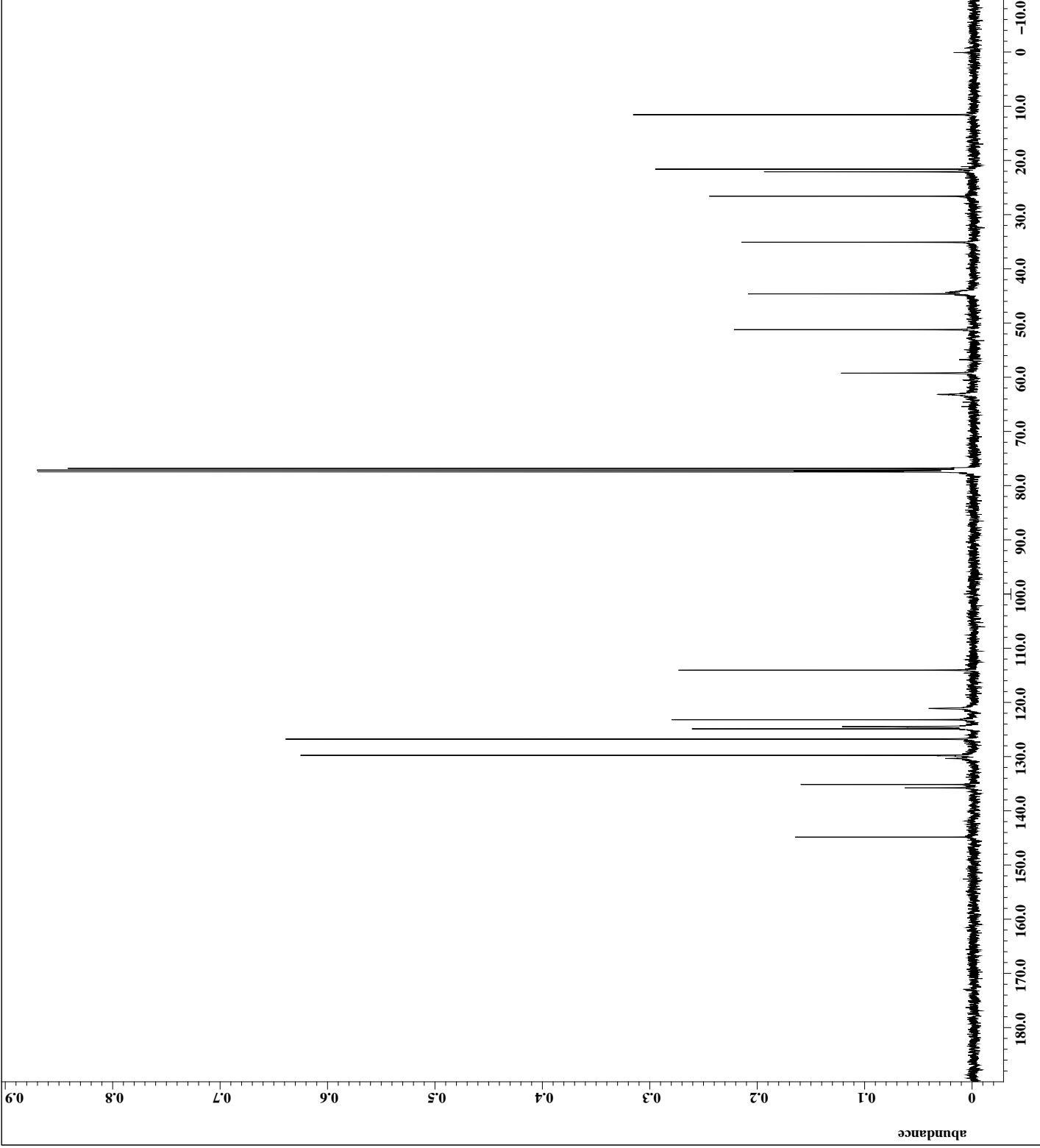
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.5[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get = 23.9[dC]

```



X : parts per Million : 1H



```

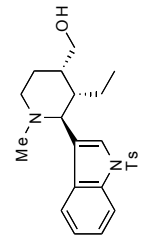
Filename = 13C alcohol isomer-2.
Author = delta
Experiment = single_pulse_dec
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 23-APR-2010 13:53:58
Revision_time = 24-AUG-2010 18:57:19
Current_time = 24-AUG-2010 18:58:27

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

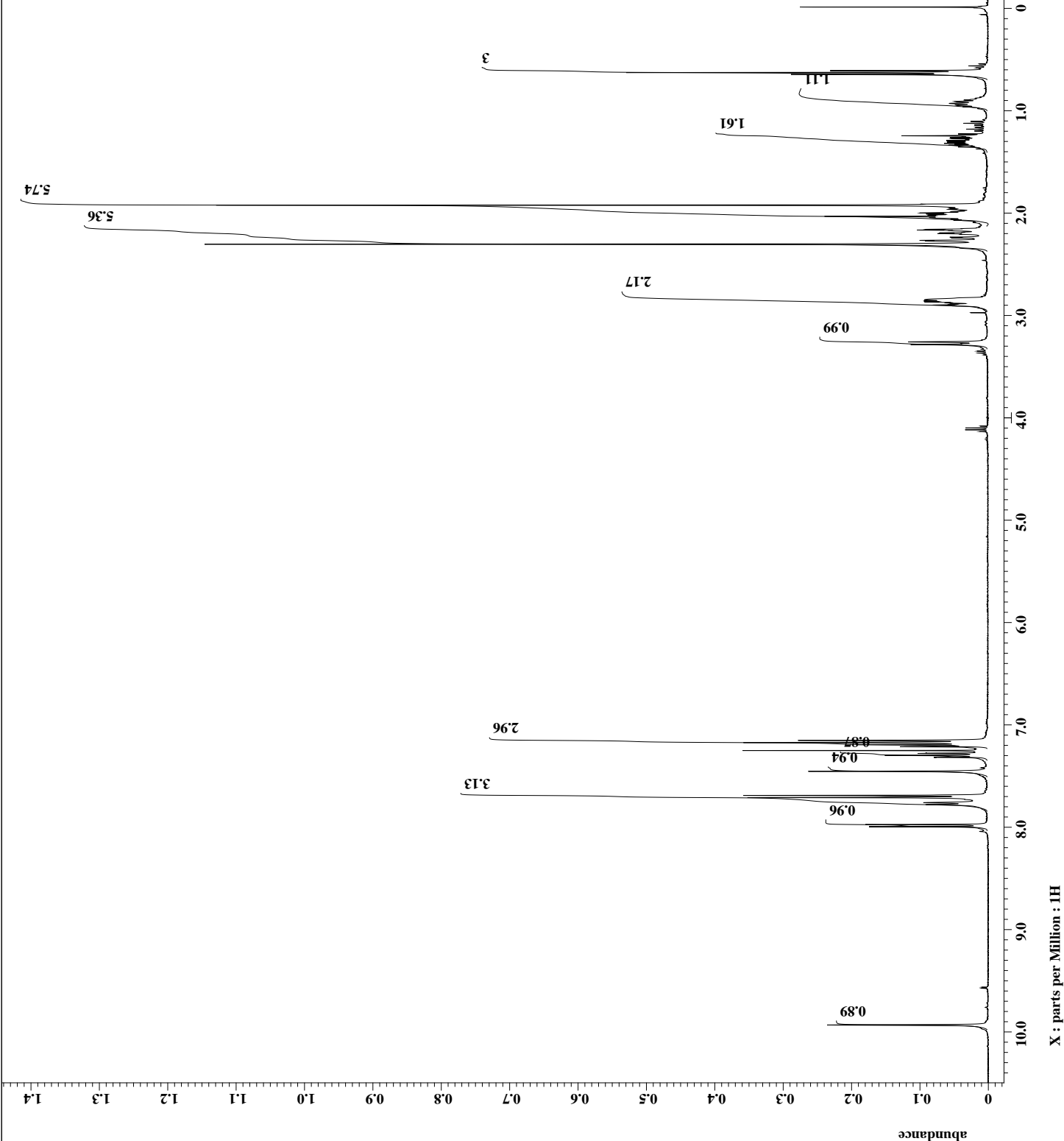
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 304
Total_scans = 304

X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[db]
X_pulse = 4.6[us]
Irr_atn_dec = 22.2[db]
Irr_atn_noe = 22.2[db]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 58
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.6[dc]

```



X : parts per Million : 13C



```

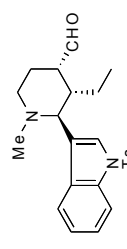
Filename = 1H Aldehyde isomer-3.
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 26-APR-2010 08:25:08
Revision_time = 24-AUG-2010 19:06:04
Current_time = 24-AUG-2010 19:06:46

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.5[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 32
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get = 23.4[dC]

```



32a

```

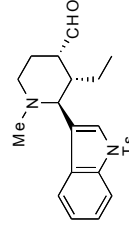
Filename = 13C Aldehyde isomer-2
Author = delta
Experiment = single_pulse_dec
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 26-APR-2010 08:50:57
Revision_time = 24-AUG-2010 19:08:13
Current_time = 24-AUG-2010 19:08:50

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

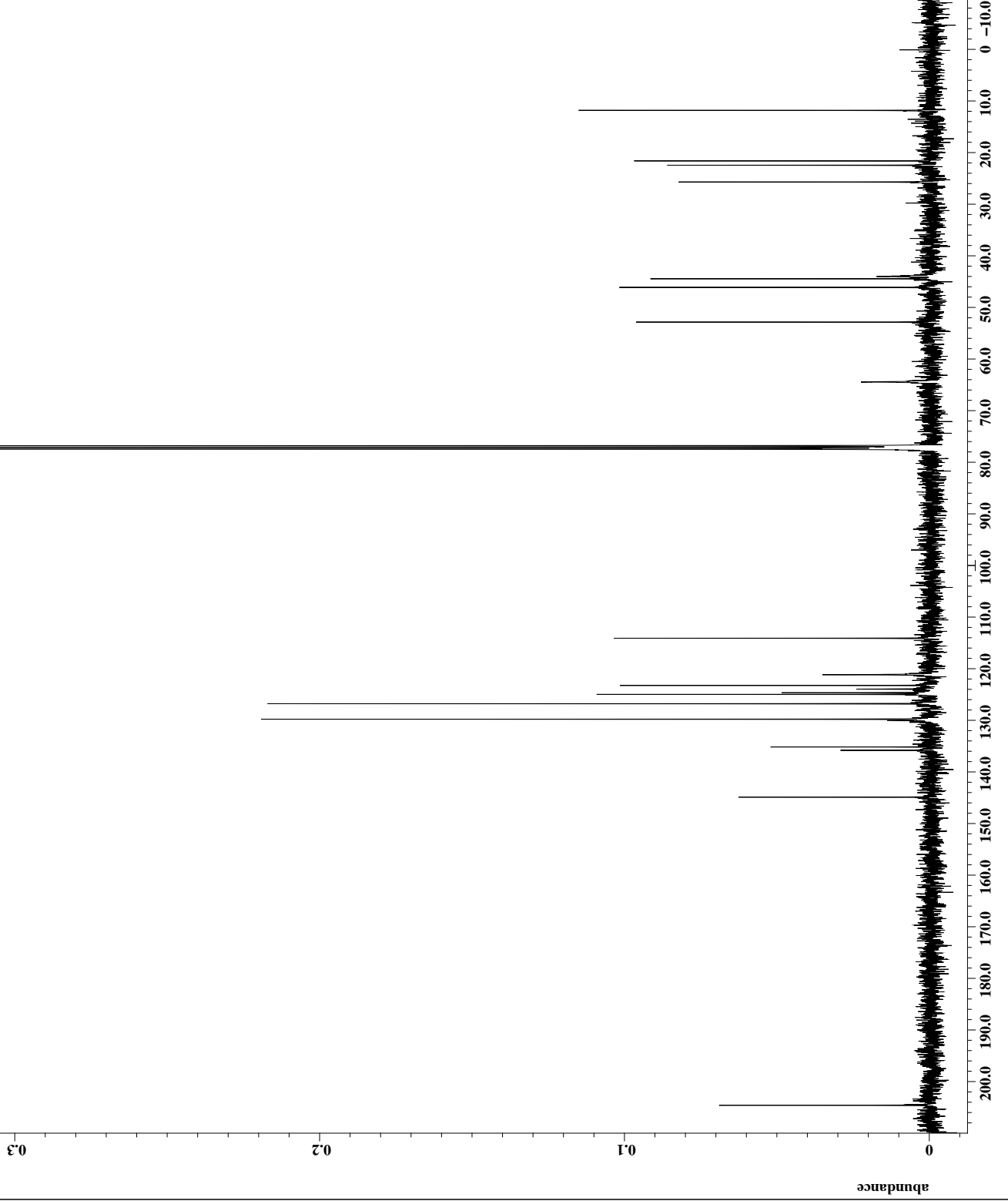
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 221
Total_scans = 221

X_90_width = 9.2[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 6.6[db]
x_pulse = 4.6[us]
Irr_atn_dec = 22.2[db]
Irr_atn_noe = 22.2[db]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 54
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24[dc]

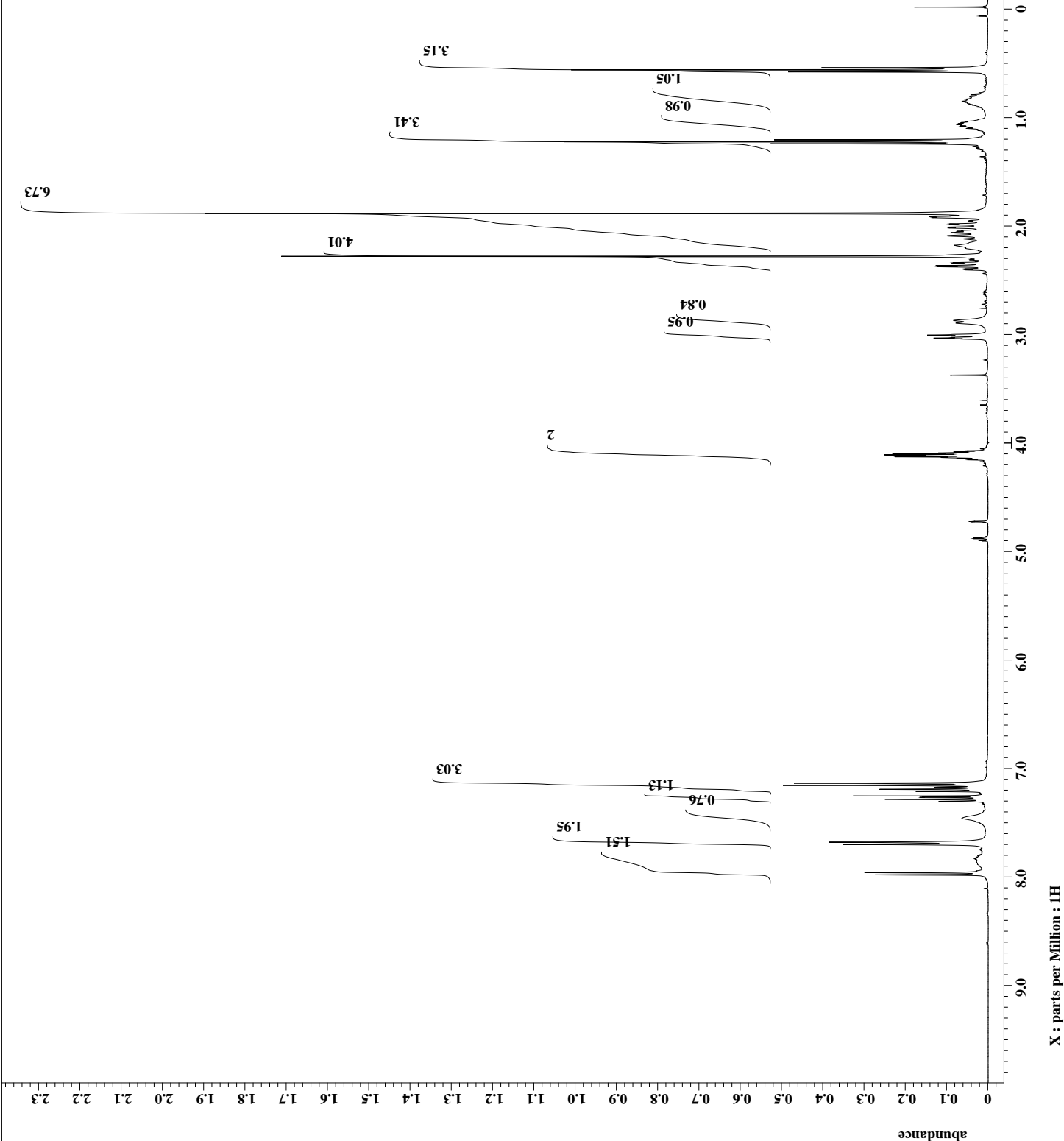
```



32a



X : parts per Million : 13C



```

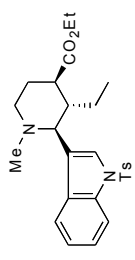
File      = 1H N-methyl-2.jdf
Name     = delta
Exp      = single_pulse.ex2
Sample   = 1
Solvent  = CHLOROFORM-D
Creation = 12-FEB-2008 16:16:09
Revision = 6-NOV-2009 17:00:56
Time     = 25-AUG-2010 17:129:26

Comment  = single_pulse
Data     = ID COMPLEX
Dim      = 26214
Title    = 1H
Units    = [ppm]
Dim1     = X
Dim2     = X
Site     = ECX400M
Spectrom = DELTA2_NMR

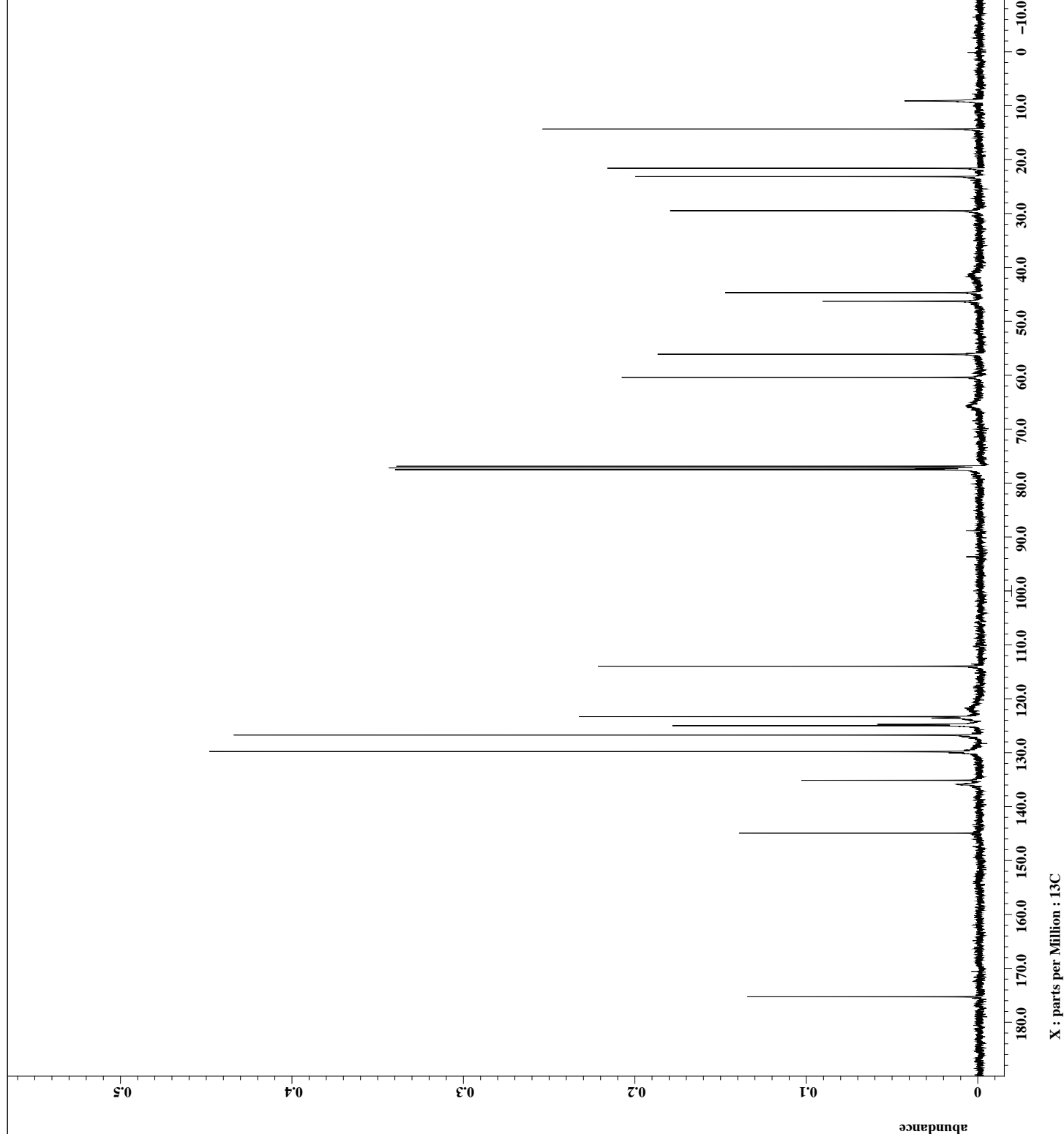
Field    = 9.389766[T] (400[MHz])
Acq      = 4.36731904[s]
Domain   = 1H
Freq     = 399.78219838[MHz]
Points   = 4[ppm]
Points   = 32768
Prescans = 1
Resol    = 0.22897343[Hz]
Sweep    = 7.5030012[KHz]
Domain   = 1H
Freq     = 399.78219838[MHz]
Offset   = 5[ppm]
Domain   = 1H
Freq     = 399.78219838[MHz]
Offset   = 5[ppm]
Clipped  = FALSE
Mod      = 1
Returns  = 8
Total    = 8

X90      = 11.2[us]
Acq      = 4.36731904[s]
Angle    = 45[deg]
Att      = 2.8[dB]
Pulse    = 5.6[us]
Mode     = Off
Dante    = FALSE
Initial  = 1[s]
Recvr    = 24
Relax    = 5[s]
Repet    = 9.36731904[s]
Temp     = 18.8[dC]

```



X : parts per Million : 1H



```

Filename = 13C N-methyl-1.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 12-FEB-2008 16:49:50
Revision_time = 12-FEB-2008 16:52:45
Current_time = 25-AUG-2010 17:30:51

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

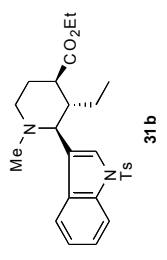
```

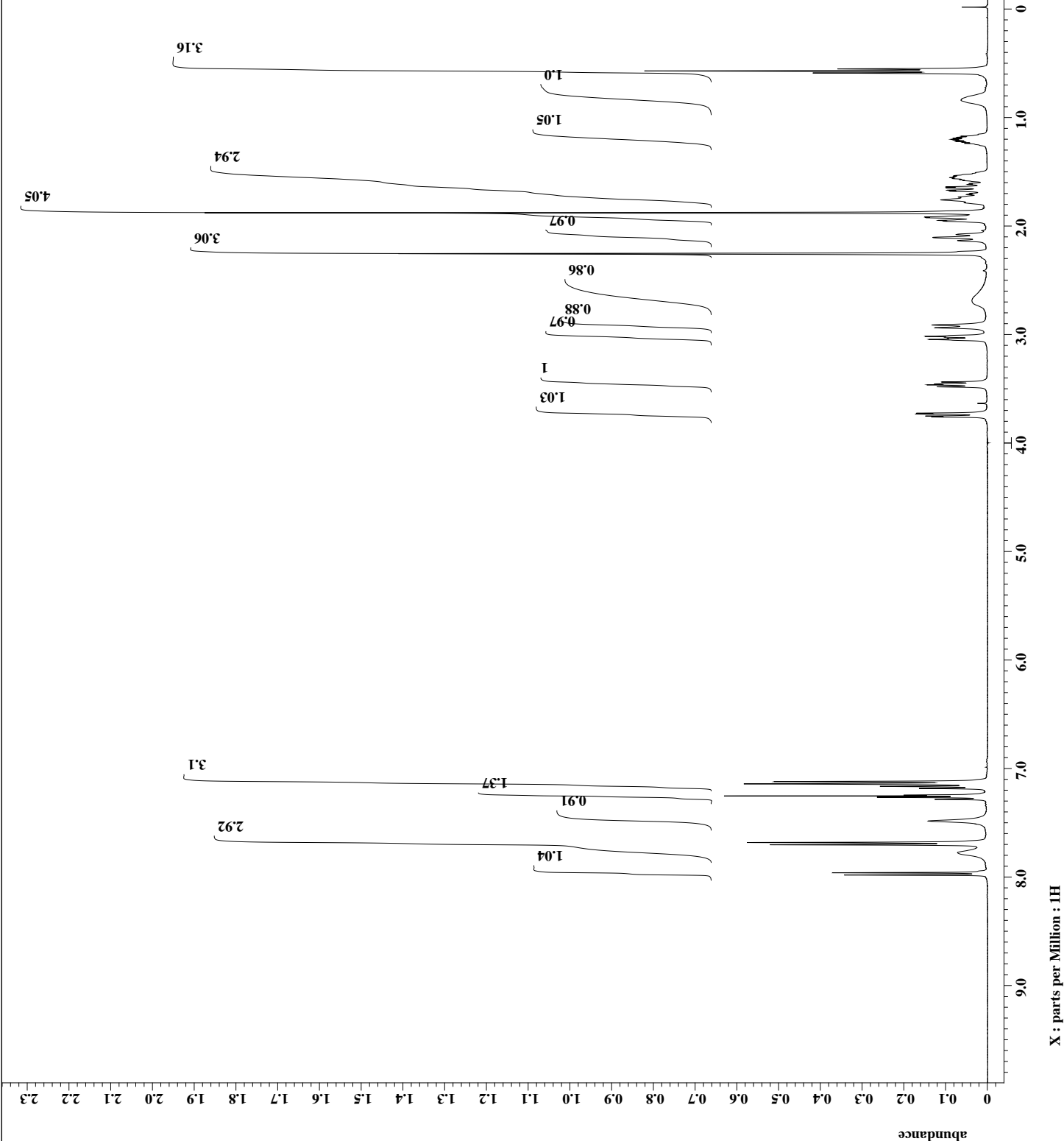
```

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 225
Total_scans = 225

X_90_width = 9.6[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 7.8[db]
X_pulse = 4.8[us]
Irr_atn_dec = 21.4[db]
Irr_atn_noe = 21.4[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 22.9[dc]

```





```

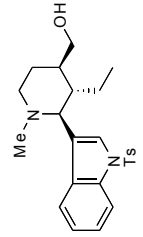
Filename = 1H alcohol-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 27-FEB-2008 12:22:16
Revision_time = 25-AUG-2010 17:31:53
Current_time = 25-AUG-2010 17:32:29

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.2[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 2.8[dB]
X_pulse = 5.6[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 20
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get = 22.5[dC]

```



X : parts per Million : 1H

```

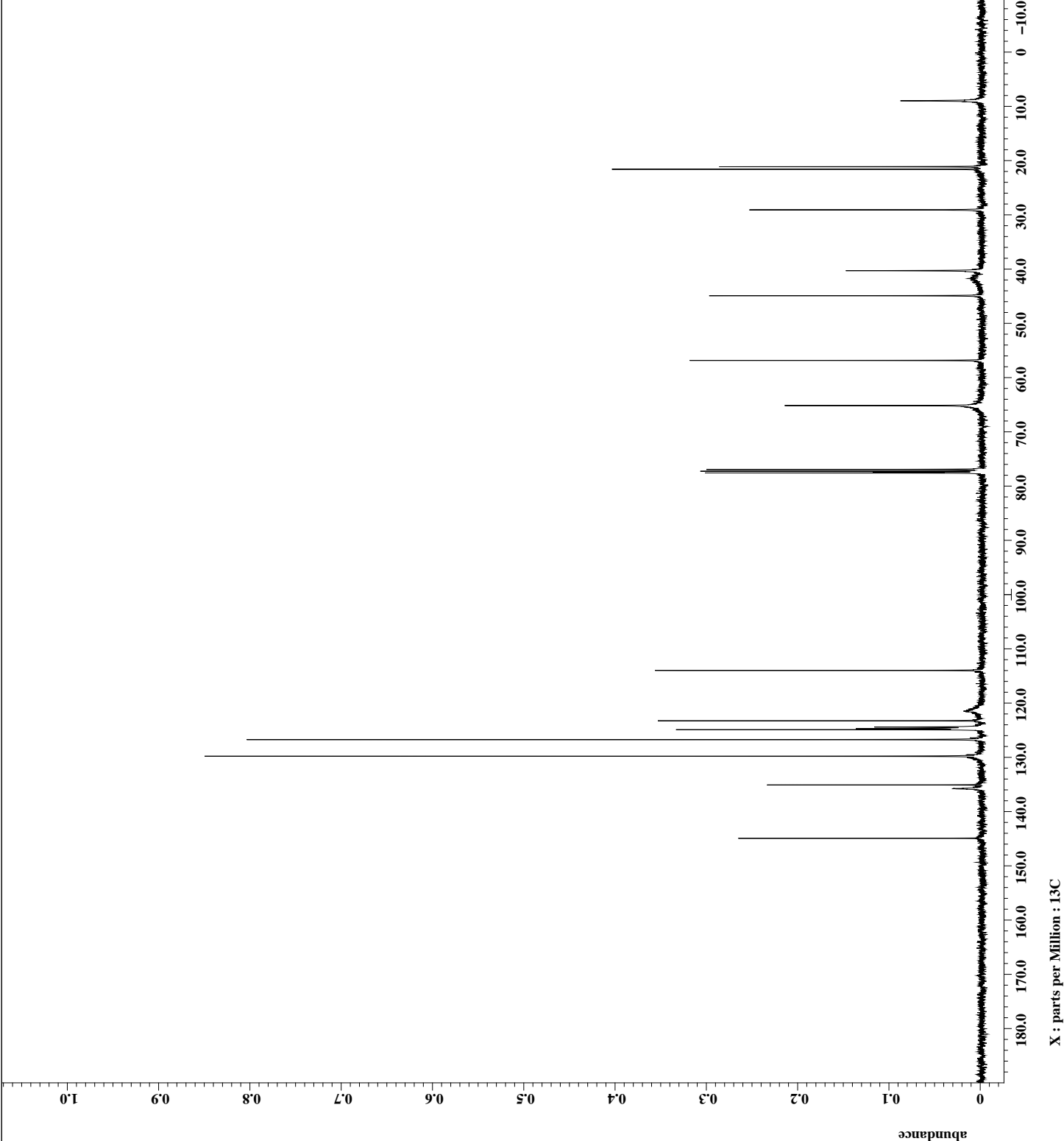
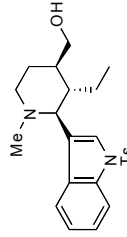
Filename = 13C alcohol-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 27-FEB-2008 12:42:15
Revision_time = 25-AUG-2010 17:32:38
Current_time = 25-AUG-2010 17:33:20

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

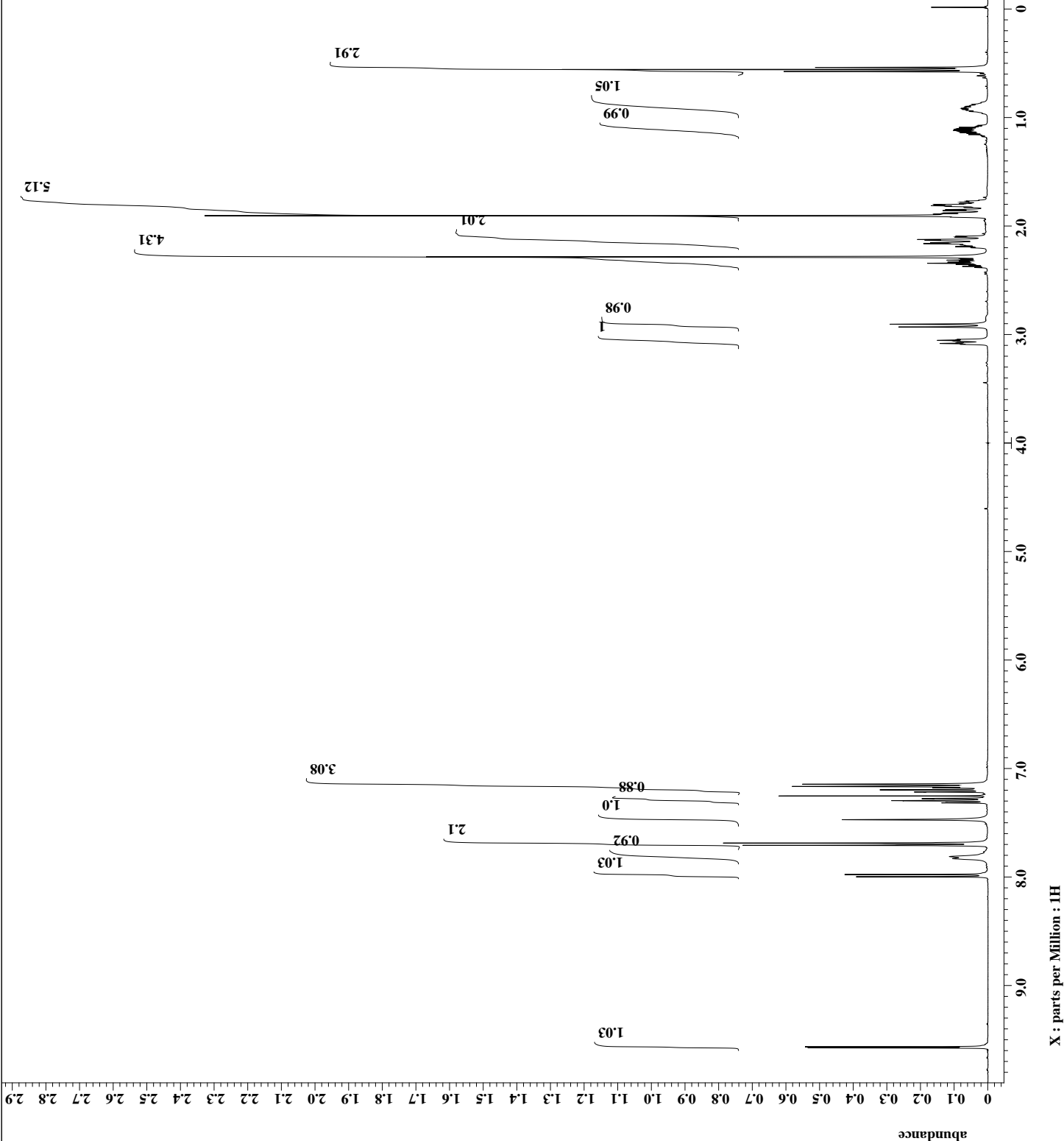
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 91
Total_scans = 91

X_90_width = 9.6[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 7.8[db]
X_pulse = 4.8[us]
Irr_atn_dec = 21.4[db]
Irr_atn_noe = 21.4[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 23.1[dc]

```



X : parts per Million : 13C



```

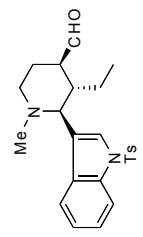
Filename = 1H aldehyde-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 3-MAR-2008 12:26:44
Revision_time = 25-AUG-2010 17:35:15
Current_time = 25-AUG-2010 17:35:26

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.2[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 2.8[dB]
X_pulse = 5.6[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 24
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get = 23.2[dC]

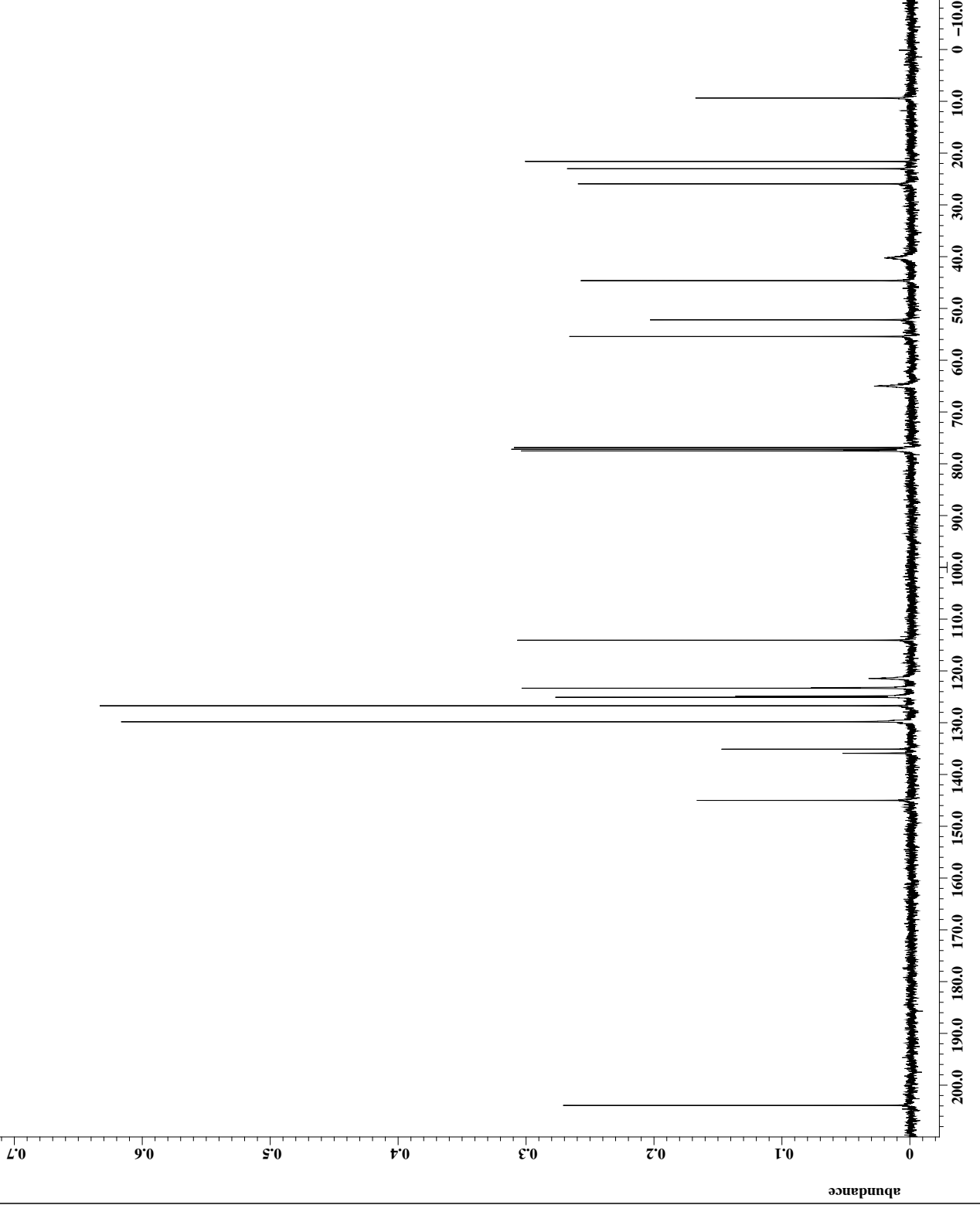
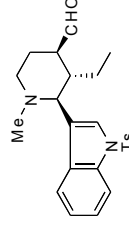
```



32b

X : parts per Million : 1H

Filename = 13C_aldehyde-2.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#453413
 Solvent = CHLOROFORM-D
 Creation_time = 3-MAR-2008 12:47:11
 Revision_time = 25-AUG-2010 17:35:32
 Current_time = 25-AUG-2010 17:35:55
 Comment = single pulse decouple
 Data_format = ID COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 82
 Total_scans = 82
 X_90_width = 9.6[us]
 X_acq_time = 1.04333312[s]
 X_angle = 45[deg]
 X_atn = 7.8[db]
 X_pulse = 4.8[us]
 Irr_atn_dec = 21.4[db]
 Irr_atn_noe = 21.4[db]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 5[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 6.04333312[s]
 Temp_get = 23.7[dc]



```

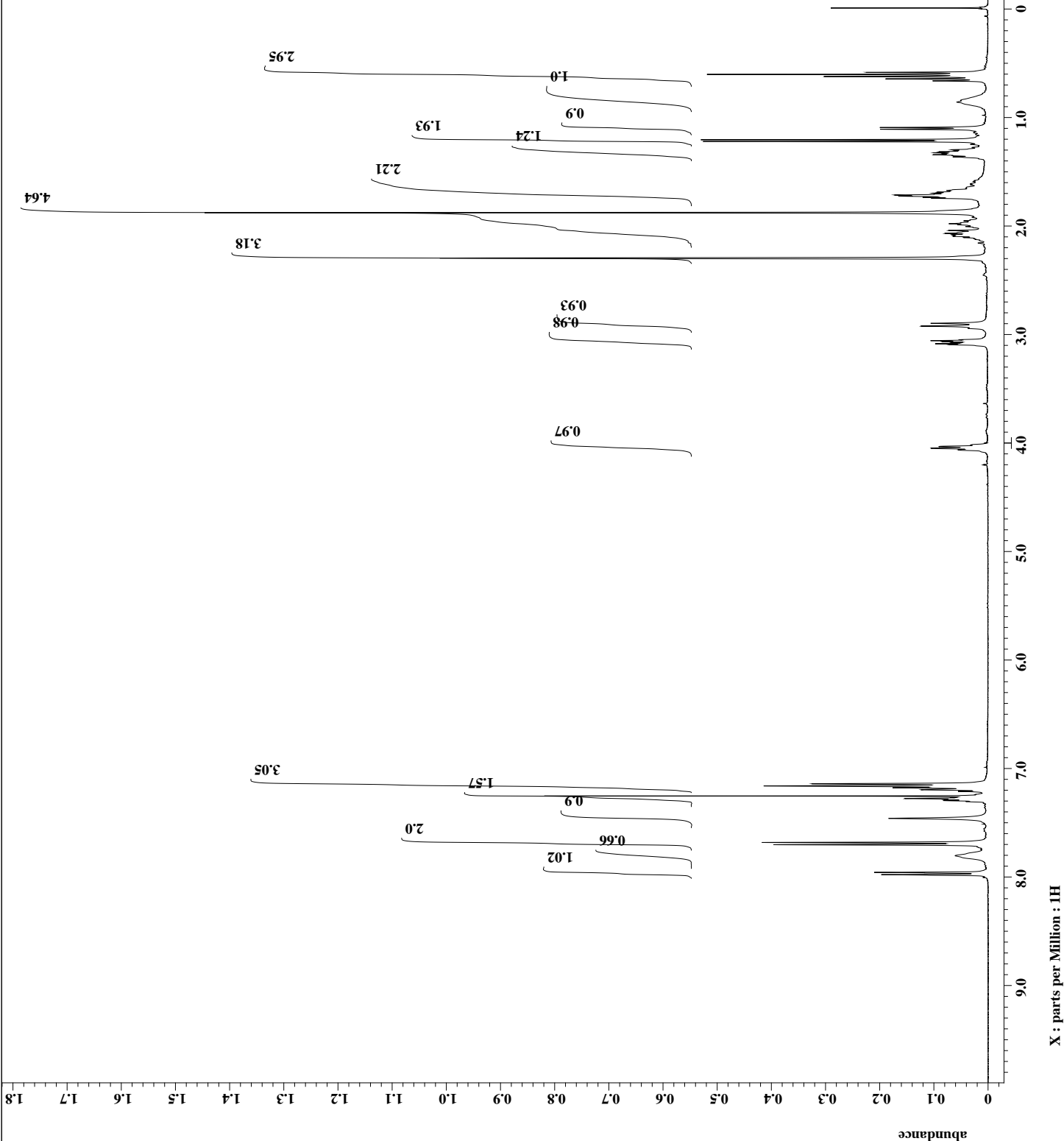
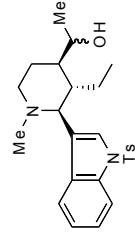
Filename = 1H secAlcohol-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 4-MAR-2008 09:38:24
Revision_time = 25-AUG-2010 17:37:27
Current_time = 25-AUG-2010 17:48:41

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.2[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 2.8[dB]
X_pulse = 5.6[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get = 23.6[degC]

```



X : parts per Million : 1H

```

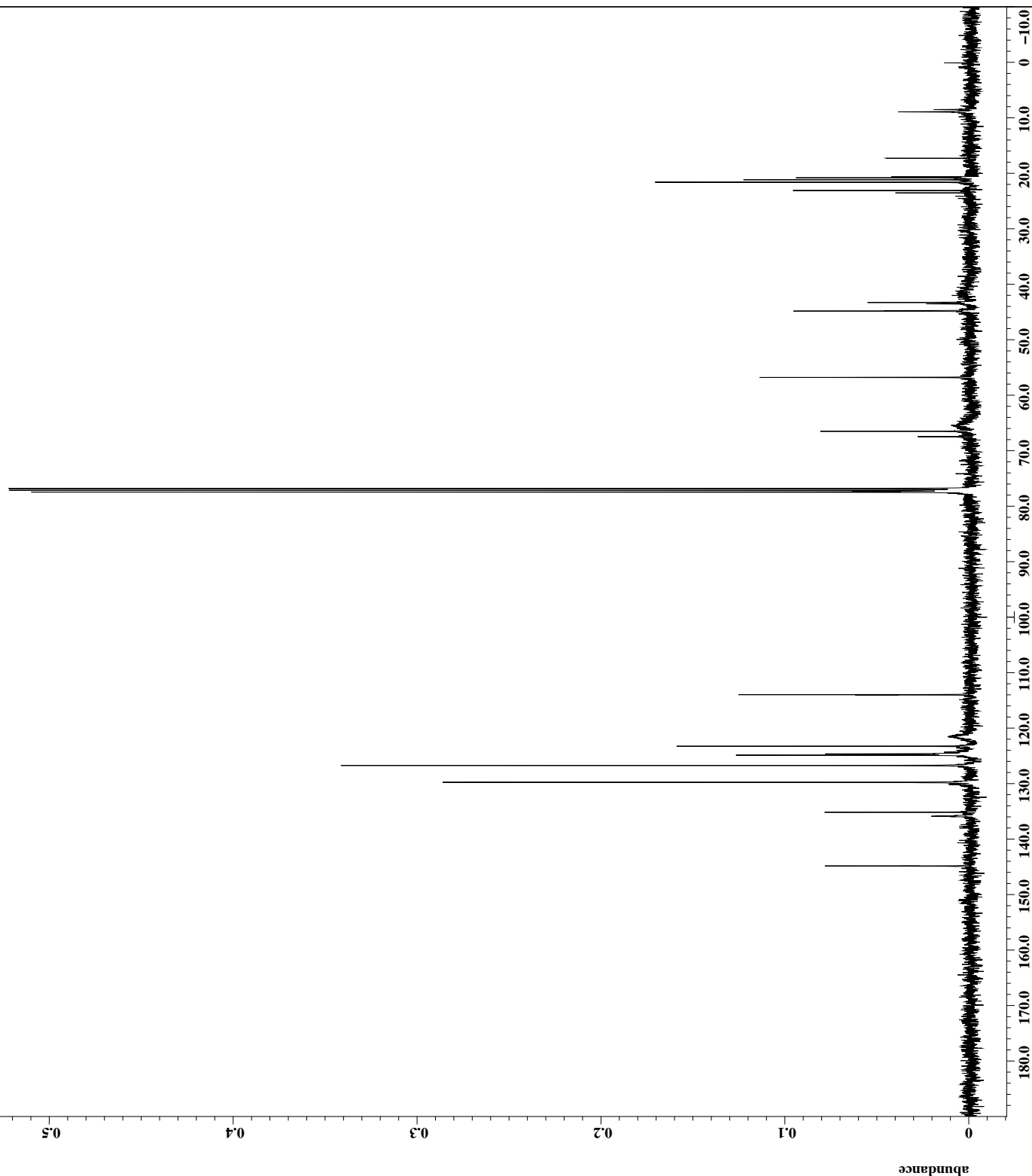
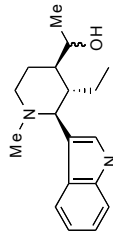
Filename = 13C_secalcohol-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 4-WAR-2008 10:07:27
Revision_time = 25-AUG-2010 17:48:50
Current_time = 25-AUG-2010 17:49:31

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

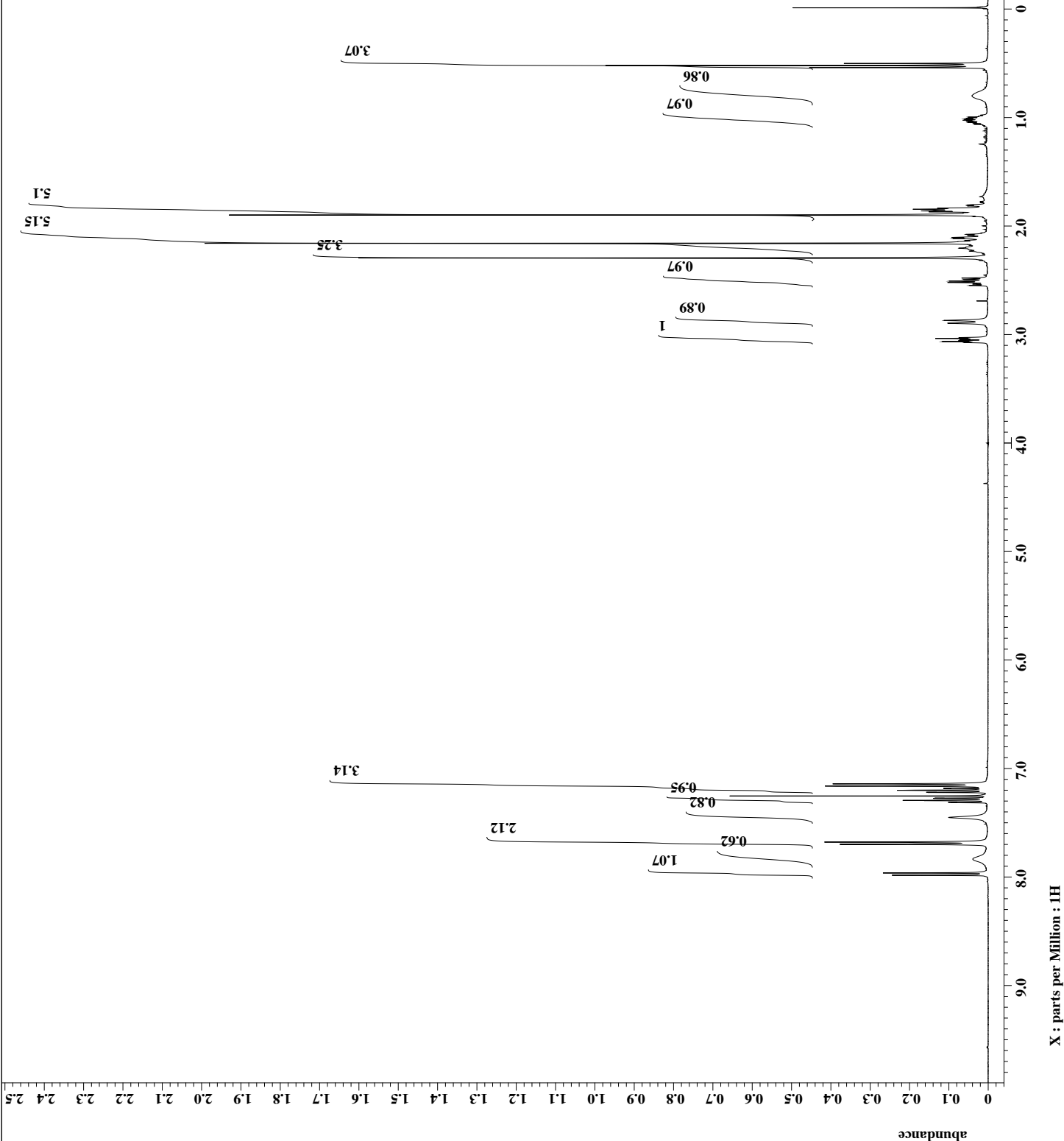
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 171
Total_scans = 171

X_90_width = 9.6[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 7.8[db]
X_pulse = 4.8[us]
Irr_atn_dec = 21.4[db]
Irr_atn_noe = 21.4[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 54
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.2[dc]

```



X : parts per Million : 13C



```

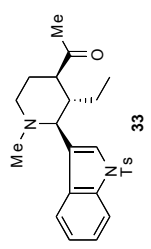
File      = 1H ketone-2.jdf
Author    = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent   = CHLOROFORM-D
Creation_time = 1-FEB-2008 10:40:07
Revision_time = 6-NOV-2009 16:50:43
Current_time = 25-AUG-2010 17:50:17

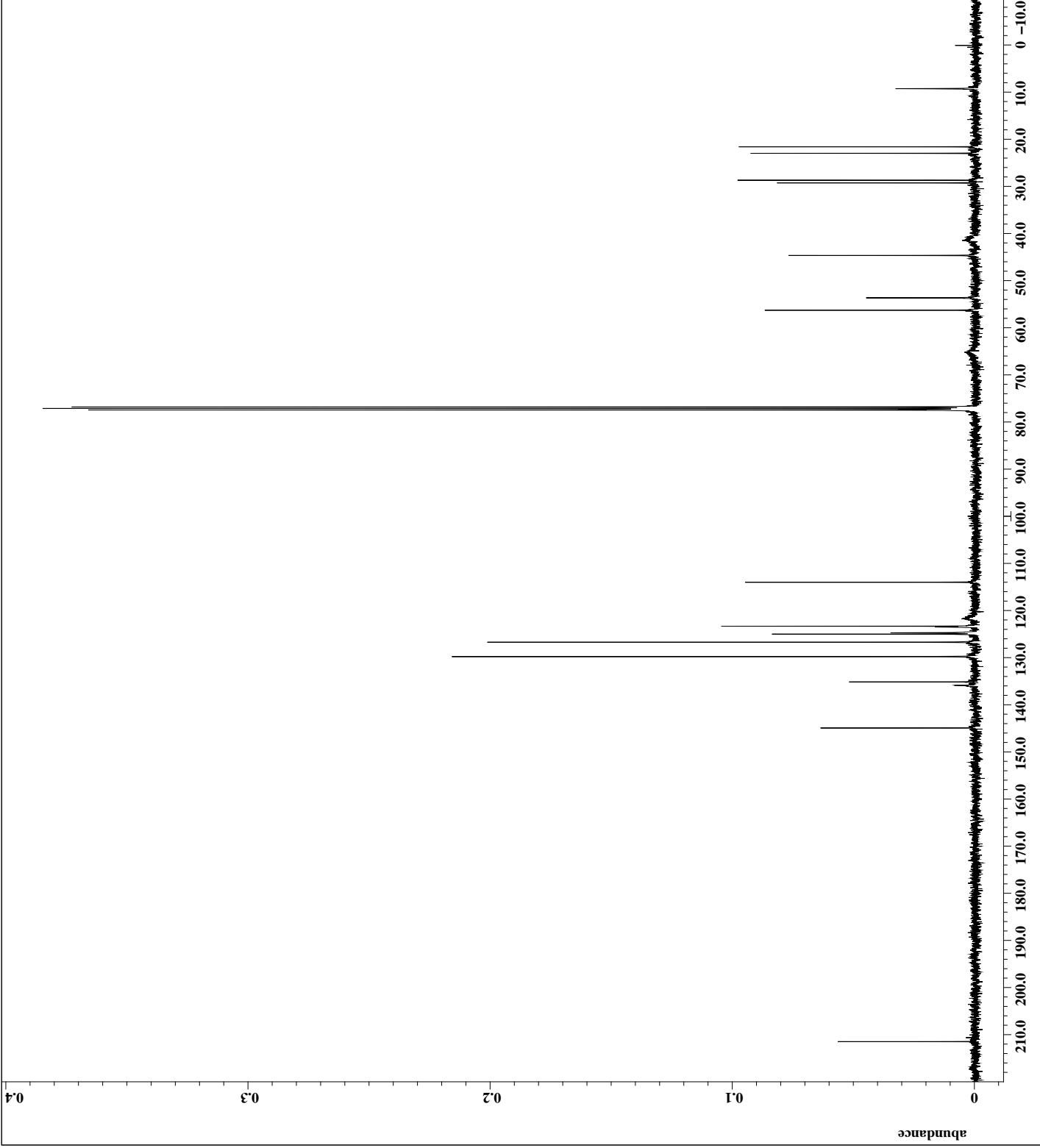
Comment   = single_pulse
Data_format = ID COMPLEX
Dim_size  = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site      = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain       = 1H
X_freq         = 399.78219838[MHz]
X_offset       = 4[ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.22897343[Hz]
X_sweep        = 7.5030012[KHz]
Irr_domain     = 1H
Irr_freq       = 399.78219838[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 399.78219838[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width     = 11.2[us]
X_acq_time     = 4.36731904[s]
X_angle        = 45[deg]
X_atn          = 2.8[dB]
X_pulse        = 5.6[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 30
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get       = 23.9[degC]

```





```

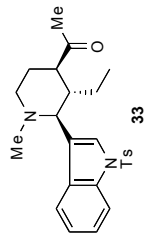
Filename = 13C ketone-1.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#391142
Solvent = CHLOROFORM-D
Creation_time = 1-FEB-2008 11:28:12
Revision_time = 1-FEB-2008 11:30:27
Current_time = 25-AUG-2010 17:50:56

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 354
Total_scans = 354

X_90_width = 9.6[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 7.8[db]
x_pulse = 4.8[us]
Irr_atn_dec = 21.4[db]
Irr_atn_noe = 21.4[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.2[dc]

```



```

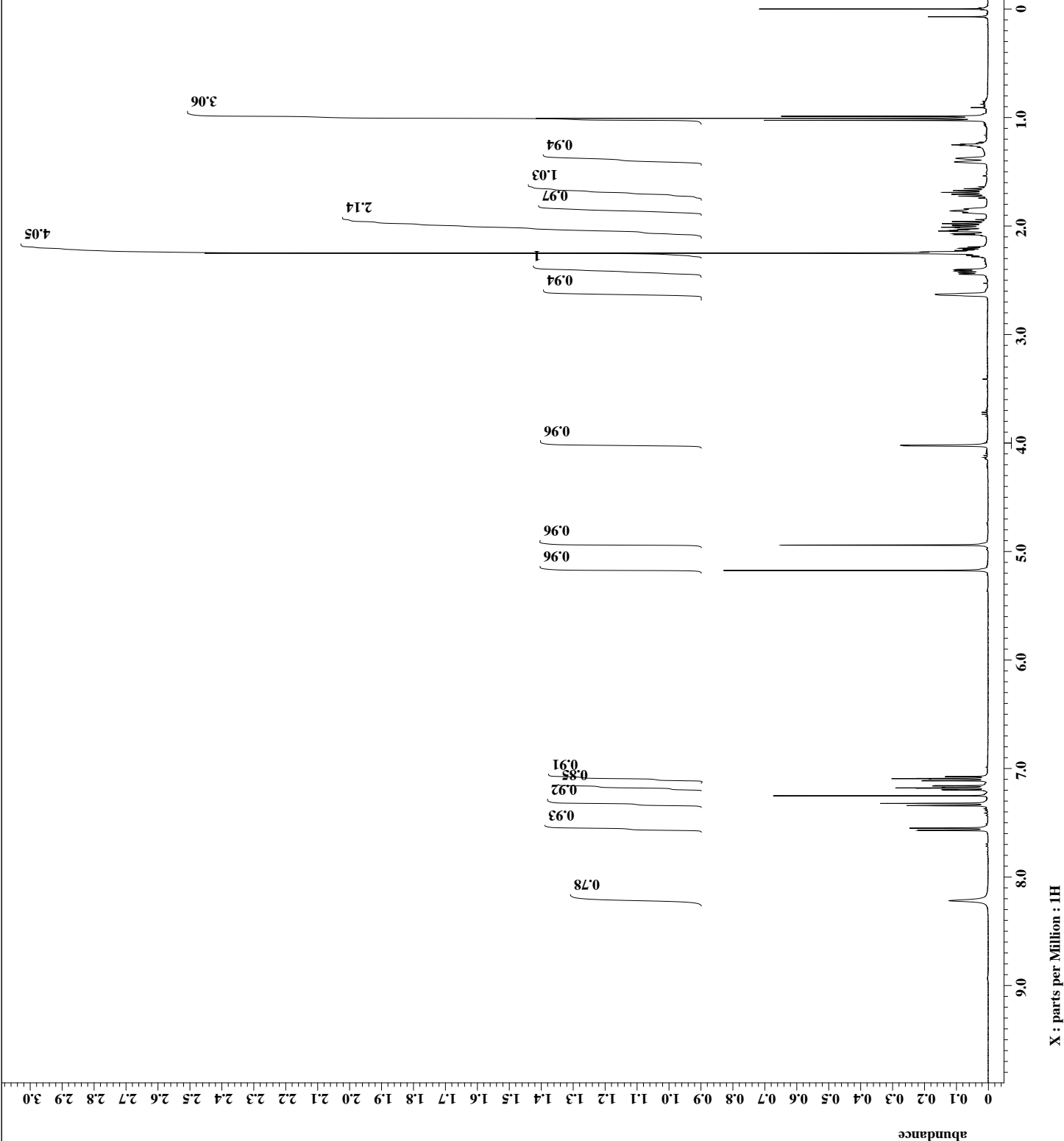
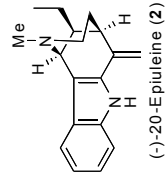
Filename = 1H 20-Epiuleine-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 7-FEB-2009 11:09:05
Revision_time = 25-AUG-2010 17:56:37
Current_time = 25-AUG-2010 17:59:10

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

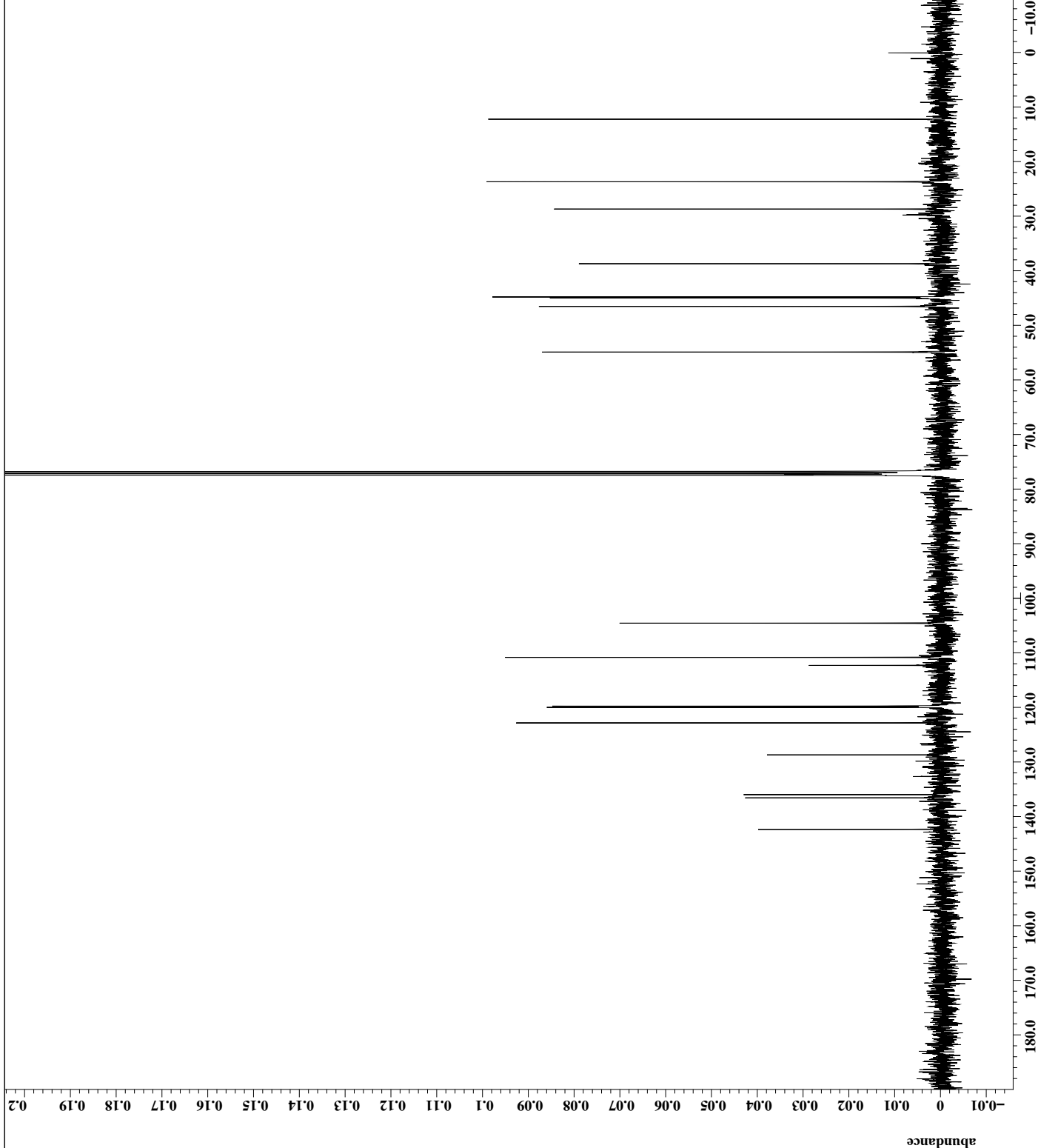
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 4.36731904[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.22897343[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_domain = 1H
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.5[us]
X_acq_time = 4.36731904[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 1[s]
Repetition_time = 5.36731904[s]
Temp_get = 24[dc]

```



X : parts per Million : 1H



```

Filename = 13C 20-Epiuleine-2.jd
Author = delta
Experiment = single_pulse_dec
Sample_id = S#438516
Solvent = CHLOROFORM-D
Creation_time = 7-FEB-2009 11:42:44
Revision_time = 25-AUG-2010 17:59:21
Current_time = 25-AUG-2010 18:00:05

Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 215
Total_scans = 215

X_90_width = 8.4[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[db]
X_pulse = 4.2[us]
Irr_atn_dec = 22.2[db]
Irr_atn_noe = 22.2[db]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 52
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.3[dc]

```

