

Concise Syntheses of Hyrtioreticulins C and D *via* a C-4 Pictet-Spengler Reaction: Revised Signs of Specific Rotations

Supporting Information

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EXPERIMENTAL

1. General Methods

Optical rotations were recorded on a JASCO P-2200 polarimeter. Melting points were recorded with a Yamato MP21 and are uncorrected. High-resolution MS spectra were recorded with a Micromass AutoSpec 3100 and a JEOL JMS-T100LP mass spectrometers. IR spectra were measured with a Shimadzu IRAffinity-1 spectrometer. The NMR experiments were performed with a JEOL JNM-ECA500 (500 MHz) spectrometer, and chemical shifts are expressed in ppm (d) with TMS as an internal reference. Column chromatography, Flash column chromatography and Medium Pressure Liquid Chromatography (MPLC) were performed on silica gel (Silica Gel 60N, Kanto Chemical Co., Ltd.). Microwave irradiation was performed with a Green-Motif I (IMCR-25003) monomode microwave reactor (IDX Corporation). All microwave irradiation experiments were carried out in glass tubes with microwave power at 50 W or 80 W.

2. Synthesis of 14, 16, and 17 (scheme 1).

Acid-promoted Pictet-Spengler reactions at room temperature:

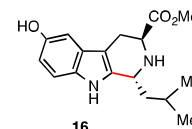
3-Methylbutanal (60 μ L, 0.6 mmol) was added to a solution of tryptophan **13** (47mg, 0.2 mmol) in MeOH (4 mL) and stirred at room temperature. After 120 h, the mixture was added to saturated NaHCO_3 solution at 0 $^\circ\text{C}$, extracted with AcOEt (50 mL), washed with brine, and dried over MgSO_4 . The solvent was removed, and the residue was purified by silica gel column chromatography with $\text{CHCl}_3/\text{MeOH}$ (2/1) to give **16** (12 mg, 20% yield) and **17** (11 mg, 18% yield).

Acid-promoted Pictet-Spengler reactions under reflux:

3-Methylbutanal (60 μ L, 0.6 mmol) was added to a solution of tryptophan **13** (47mg, 0.2 mmol) in MeOH (4 mL) and stirred for 48 h under reflux. After the mixture had cooled, the mixture was added to saturated NaHCO_3 solution at 0 $^\circ\text{C}$, extracted with AcOEt (50 mL), washed with brine, and dried over MgSO_4 . The solvent was removed, and the residue was purified by silica gel column chromatography with $\text{CHCl}_3/\text{MeOH}$ (2/1) to give **14** (8 mg, 14% yield), **16** (29 mg, 48% yield), and **17** (14 mg, 23% yield).

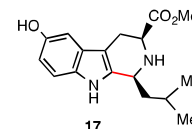
Methyl (1*R*,3*S*)-6-hydroxy-1-isobutyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**16**).

14 mg, 23% yield, an amorphous white powder. $[\alpha]_D^{24} = +26.2$ ($c = 0.10$ in MeOH). Mp: 114-117 $^\circ\text{C}$ ($\text{CHCl}_3/\text{MeOH}$). IR (CHCl_3): 3471, 1734 cm^{-1} . $^1\text{H-NMR}$ ($\text{DMSO-}d_6$) δ : 0.98, 0.99, 1.01, 1.02 (4 s, 6H), 1.49 (dd, $J = 4.6, 9.5$ Hz, 1H), 1.70 (dd, $J = 4.6, 9.8$ Hz, 1H), 1.92 (m, 1H), 2.88 (dd, $J = 7.5, 15.5$ Hz, 1H), 2.99 (dd, $J = 5.2, 15.5$ Hz, 1H), 3.75 (s, 3H), 3.95 (dd, $J = 5.2, 7.5$ Hz, 1H), 4.26 (dd, $J = 4.1, 9.8$ Hz, 1H), 6.69 (dd, $J = 2.3, 8.6$ Hz, 1H), 6.84 (d, $J = 2.3$ Hz, 1H), 7.11 (d, $J = 8.6$ Hz, 1H), 7.25 (br s, 1H), 7.58 (br s, 1H). $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$) δ : 21.8, 23.7, 24.8, 25.0, 44.5, 48.3, 52.3, 52.5, 103.1, 106.5, 111.2, 111.3, 128.0, 131.1, 137.2, 149.6, 174.3. HR-EI-MS m/z : Calcd for $\text{C}_{17}\text{H}_{22}\text{N}_2\text{O}_3$ [M^+]: 302.1630. Found 302.1632.



Methyl (1*S*,3*S*)-6-hydroxy-1-isobutyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**17**).

29 mg, 48% yield, an amorphous white powder. $[\alpha]_D^{24} = -71.1$ ($c = 0.10$ in MeOH). Mp: 154-156 $^\circ\text{C}$ ($\text{CHCl}_3/\text{MeOH}$). IR (CHCl_3): 3480, 1718 cm^{-1} . $^1\text{H-NMR}$ ($\text{DMSO-}d_6$) δ : 0.89 (d, $J = 6.9$ Hz, 3H), 0.93 (d, $J = 6.9$ Hz, 3H), 1.42 (ddd, $J = 2.9, 9.8, 13.7$ Hz, 1H), 1.76 (ddd, $J = 2.9, 9.8, 13.7$ Hz, 1H), 1.87 (m, 1H), 2.53 (ddd, $J = 1.7, 12.1, 13.7$ Hz, 1H), 2.77 (dd, $J = 2.9, 14.3$ Hz, 1H), 3.62 (dd, $J = 4.0, 10.9$ Hz, 1H), 3.67 (s, 3H), 4.01 (d, $J = 9.8$ Hz, 1H), 6.48 (dd, $J = 1.8, 8.1$ Hz, 1H), 6.62 (d, $J = 2.3$ Hz, 1H), 7.02 (d, $J = 8.6$ Hz, 1H), 8.55 (br s, 1H), 10.36 (br s, 1H). $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$) δ : 22.0, 24.2, 24.5, 26.3, 43.6, 51.0, 52.2, 56.7, 102.2, 105.6, 110.9, 111.8, 128.0, 130.8, 138.2, 150.8, 174.1. HR-EI-MS m/z : Calcd for $\text{C}_{17}\text{H}_{22}\text{N}_2\text{O}_3$ [M^+]: 302.1630. Found 302.1631.

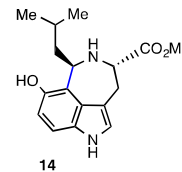


Base-promoted Pictet-Spengler reaction:

3-Methylbutanal (60 μ L, 0.6 mmol) was added to a solution of tryptophan **13** (47mg, 0.2 mmol) in Et₃N/MeOH (1/1, v/v, 4 mL) and stirred for 48 h under reflux. After the mixture had cooled, the mixture was added to saturated NaHCO₃ solution at 0 °C, extracted with AcOEt (50 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was purified by silica gel column chromatography with CHCl₃/MeOH (2/1) to give **14** (41 mg, 67% yield).

methyl (1*R*,3*S*)-9-hydroxy-1-isobutyl-2,3,4,6-tetrahydro-1*H*-azepino[5,4,3-*cd*]indole-3-carboxylate (14**).**

41 mg, 67% yield, an amorphous white powder. $[\alpha]_D^{24} = -22.8$ ($c = 0.10$ in MeOH). Mp: 171-173 °C (CHCl₃/MeOH). IR (CHCl₃): 3480, 1718 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 1.48 (d, $J = 6.9$ Hz, 3H), 2.79 (t, $J = 13.7$ Hz, 1H), 3.28 (dd, $J = 2.3, 15.5$ Hz, 1H), 3.65 (s, 3H), 3.82 (dd, $J = 2.3, 12.0$ Hz, 1H), 4.58 (dd, $J = 3.5, 11.5$ Hz, 1H), 6.55 (dd, $J = 8.6$ Hz, 1H), 6.92 (d, $J = 8.6$ Hz, 1H), 6.97 (s, 1H), 8.38 (br s, 1H), 10.50 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 21.4, 24.6, 24.7, 34.8, 40.8, 52.3, 53.3, 54.0, 109.4, 111.4, 111.8, 123.0, 124.8, 125.7, 132.2, 145.2, 175.2. HR-EI-MS m/z : Calcd for C₁₇H₂₂N₂O₃ [M^+]: 302.1630. Found 302.1637.



3. Synthesis of **20** and **21** (Table 1).

Acid-promoted Pictet-Spengler reaction at room temperature (entry 3):

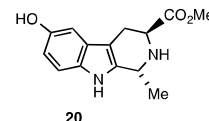
Acetaldehyde (0.17 mL, 3 mmol) was added to a solution of tryptophan **13** (234 mg, 1 mmol) in AcOH/MeOH (1/10, v/v, 10 mL) and stirred at room temperature. After 1.5 h, the mixture was added to saturated NaHCO₃ solution at 0 °C, extracted with AcOEt (100 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was purified by silica gel column chromatography with CHCl₃/MeOH (2/1) to give **20** (45 mg, 17% yield) and **21** (150 mg, 58% yield).

Acid-promoted Pictet-Spengler reaction at 50 °C (entry 4):

Acetaldehyde (0.17 mL, 3 mmol) was added to a solution of tryptophan **13** (234 mg, 1 mmol) in AcOH/MeOH (1/10, v/v, 10 mL) at room temperature and stirred for 1 h at 50 °C. After the mixture had cooled, the mixture was added to saturated NaHCO₃ solution at 0 °C, extracted with AcOEt (100 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was purified by silica gel column chromatography with CHCl₃/MeOH (2/1) to give **20** (42 mg, 16% yield) and **21** (105 mg, 40% yield).

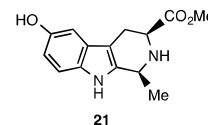
Methyl (1*R*,3*S*)-6-hydroxy-1-methyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**16**).¹

45 mg, 17% yield (entry 3, table 1), an amorphous white powder. $[\alpha]_D^{24} = +18.2$ ($c = 0.11$ in MeOH). Mp: 104-107 °C (CHCl₃/MeOH). IR (CHCl₃): 3471, 1736 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 1.43 (d, $J = 6.9$ Hz, 3H), 2.89 (ddd, $J = 1.2, 6.9, 15.5$ Hz, 1H), 2.98 (ddd, $J = 1.2, 5.5, 15.5$ Hz, 1H), 3.71 (s, 3H), 3.96 (t, $J = 5.5$ Hz, 1H), 4.33 (q, $J = 6.9$ Hz, 1H), 6.59 (dd, $J = 2.3, 8.6$ Hz, 1H), 6.75 (d, $J = 2.3$ Hz, 1H), 7.06 (d, $J = 8.6$ Hz, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 19.7, 24.2, 45.7, 51.2, 52.3, 101.8, 104.2, 110.4, 110.9, 127.6, 131.4, 136.8, 149.9, 173.9. HR-ESI-MS m/z : Calcd for C₁₄H₁₇N₂O₃ [(M+H)⁺]: 261.1239. Found 261.1239.



Methyl (1*S*,3*S*)-6-hydroxy-1-methyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**17**).²

150 mg, 58% yield (entry 3, table 1), an amorphous white powder. $[\alpha]_D^{24} = -54.5$ ($c = 0.11$ in MeOH). Mp: 172-174 °C (CHCl₃/MeOH). IR (CHCl₃): 3472, 1735 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 1.32 (d, $J = 6.3$ Hz, 3H), 2.54 (ddd, $J = 1.7, 14.9, 14.9$ Hz, 1H), 2.76 (dd, $J = 2.9, 14.9$ Hz, 1H), 3.63 (dd, $J = 4.0, 10.9$ Hz, 1H), 4.03 (q, $J = 6.9$ Hz, 1H), 6.49 (dd, $J = 2.3, 8.6$ Hz, 1H), 6.63 (d, $J = 2.3$ Hz, 1H), 7.03 (d, $J = 8.6$ Hz, 1H), 8.58 (br s, 1H), 10.41 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 20.5, 26.1, 48.8, 52.2, 56.7, 102.3, 105.3, 110.9, 111.8, 128.0, 130.8, 138.7, 150.8, 173.8. HR-ESI-MS m/z : Calcd for C₁₄H₁₆NaN₂O₃ [(M+Na)⁺]: 283.1059. Found 283.1055.



4. Synthesis of 18 and 19 (Table 1).

Base-promoted Pictet-Spengler reactions under microwave irradiation (entry 7):

Acetaldehyde (0.17 mL, 3 mmol) was added to a solution of tryptophan **13** (234 mg, 1 mmol) in Et₃N/MeOH (1/1, v/v, 10 mL) and stirred for 5 min at room temperature. Then, the mixture was heated under reflux for 6 h using microwave irradiation (50 W). After the mixture had cooled, the mixture was evaporated. The residue was purified by silica gel column chromatography with CHCl₃/MeOH (2/1) to give **18** (84 mg, 32% yield) and **19** (45 mg, 17% yield).

Changing MeOH to EtOH (entry 8):

Acetaldehyde (0.17 mL, 3 mmol) was added to a solution of tryptophan **13** (234 mg, 1 mmol) in Et₃N/EtOH (1/1, v/v, 10 mL) and stirred for 5 min at room temperature. Then, the mixture was heated under reflux for 6 h using microwave irradiation (50 W). After the mixture had cooled, the mixture was evaporated. The residue was purified by silica gel column chromatography with CHCl₃/MeOH (2/1) to give **18** (45 mg, 17% yield), **19** (31 mg, 12% yield), **20** (48 mg, 18% yield), and **21** (28 mg, 11% yield).

Changing Et₃N to *N,N*-diisopropylethylamine (entry 9):

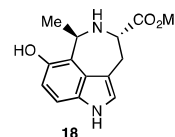
Acetaldehyde (0.17 mL, 3 mmol) was added to a solution of tryptophan **13** (234 mg, 1 mmol) in DIEA/MeOH (1/1, v/v, 10 mL) and stirred for 5 min at room temperature. Then, the mixture was heated under reflux for 6 h using microwave irradiation (50 W). After the mixture had cooled, the mixture was evaporated. The residue was purified by silica gel column chromatography with CHCl₃/MeOH (2/1) to give **18** (121 mg, 46% yield) and **19** (27 mg, 10% yield).

Changing 50W to 80W in microwave irradiation (entry 10):

Acetaldehyde (0.17 mL, 3 mmol) was added to a solution of tryptophan **13** (234 mg, 1 mmol) in DIEA/MeOH (1/1, v/v, 10 mL) and stirred for 5 min at room temperature. Then, the mixture was heated under reflux for 6 h using microwave irradiation (80 W). After the mixture had cooled, the mixture was evaporated. The residue was purified by silica gel column chromatography with CHCl₃/MeOH (2/1) to give **18** (154 mg, 59% yield) and **19** (10 mg, 4% yield).

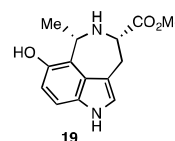
Methyl (1*R*,3*S*)-9-hydroxy-1-methyl-2,3,4,6-tetrahydro-1*H*-azepino[5,4,3-*cd*]indole-3-carboxylate (**18**).

154 mg, 59% yield (entry 10, table 1), an amorphous white powder. $[\alpha]_D^{24} = -5.0$ ($c = 0.49$ in MeOH). Mp: 183-185 °C (CHCl₃/MeOH). IR (CHCl₃): 3468, 1726, 1711 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 1.29 (d, $J = 6.9$ Hz, 3H), 2.82 (ddd, $J = 1.7, 12.6, 14.9$ Hz, 1H), 3.27 (dd, $J = 2.3, 14.9$ Hz, 1H), 3.64 (s, 3H), 3.90 (dd, $J = 1.7, 12.6$ Hz, 1H), 4.65 (q, $J = 6.9$ Hz, 1H), 6.57 (d, $J = 8.6$ Hz, 1H), 6.93 (d, $J = 8.6$ Hz, 1H), 6.98 (s, 1H), 8.41 (br s, 1H), 10.52 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 20.1, 34.7, 51.3, 52.2, 54.4, 109.5, 111.4, 111.7, 123.0, 124.9, 125.4, 132.2, 145.5, 175.1. HR-ESI-MS m/z : Calcd for C₁₄H₁₆NaN₂O₃ [(M+Na)⁺]: 283.1059. Found 283.1056.



Methyl (1*S*,3*S*)-9-hydroxy-1-methyl-2,3,4,6-tetrahydro-1*H*-azepino[5,4,3-*cd*]indole-3-carboxylate (**19**).

10 mg, 4% yield (entry 10, table 1), an amorphous white powder. $[\alpha]_D^{24} = -31.9$ ($c = 0.50$ in MeOH). Mp: 80-83 °C (CHCl₃/MeOH). IR (CHCl₃): 3346, 1734 cm⁻¹. ¹H-NMR (CDCl₃) δ : 1.61 (d, $J = 6.3$ Hz, 3H), 3.16 (ddd, $J = 1.7, 12.0, 15.5$ Hz, 1H), 3.36 (dd, $J = 2.9, 14.9$ Hz, 1H), 3.77 (s, 3H), 3.86 (dd, $J = 2.9, 12.0$ Hz, 1H), 4.65 (q, $J = 6.3$ Hz, 1H), 6.62 (d, $J = 8.6$ Hz, 1H), 6.95 (s, 1H), 7.03 (d, $J = 8.0$ Hz, 1H), 7.26 (br s, 1H), 8.02 (br s, 1H). ¹³C-NMR (CDCl₃) δ : 23.3, 34.5, 52.4, 54.1, 59.2, 109.5, 112.9, 113.0, 122.7, 124.0, 125.9, 132.6, 145.7, 175.1. HR-ESI-MS m/z : Calcd for C₁₄H₁₇N₂O₃ [(M+H)⁺]: 261.1239. Found 261.1238.



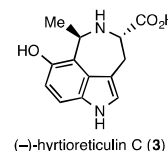
5. Synthesis of 3-6 (scheme 3).

Typical procedure for hydrolysis: 10% NaOH (0.25 mL) was added to a solution of methyl ester (0.1 mmol) in MeOH (1 mL) at room temperature, and the mixture was stirred at room temperature. After 15 min or 30 min, oxalic acid•2H₂O (63 mg, 0.5 mmol) was added to the mixture and stirred for 10 min at room temperature. The mixture was passed through Celite and the residue was washed with MeOH. The solvent was removed, and the residue was purified by silica gel column chromatography with CHCl₃/MeOH (2/1) to give the carboxylic acid.

Hyrtioreticuline C (3).³

According to the typical procedure for hydrolysis, **3** (18 mg, 72% yield) was obtained as an amorphous white powder.

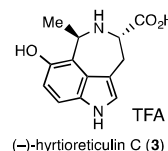
18 mg, 72% yield, an amorphous white powder. $[\alpha]_D^{24} = -86.4$ ($c = 0.10$ in MeOH). Mp: 230-232 °C (CHCl₃/MeOH). IR (CHCl₃): 3466, 1710 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 1.41 (d, $J = 6.9$ Hz, 3H), 2.87 (dd, $J = 12.6, 16.1$ Hz, 1H), 3.61 (dd, $J = 2.9, 16.7$ Hz, 1H), 3.75 (dd, $J = 2.9, 12.6$ Hz, 1H), 5.10 (q, $J = 6.9$ Hz, 1H), 6.68 (d, $J = 8.6$ Hz, 1H), 7.09 (d, $J = 8.6$ Hz, 1H), 7.10 (s, 1H), 8.90 (br s, 2H), 10.71 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 17.1, 29.4, 51.8, 56.6, 110.6, 111.4, 111.7, 116.0, 123.6, 124.7, 132.0, 146.4, 169.7. HR-ESI-MS m/z : Calcd for C₁₃H₁₄NaN₂O₃ [(M+Na)⁺]: 269.0902. Found 269.0901.



Hyrtioreticuline C (3).

Adding TFA (1 drop) into NMR tube, then ¹H and ¹³C-NMR experiments were performed. Adding TFA (1 μ L) into optical rotation cell, then specific rotation experiment was performed.

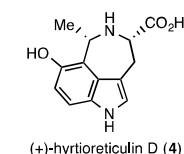
$[\alpha]_D^{24} = -60.5$ ($c = 0.10$ in MeOH-TFA). ¹H-NMR (DMSO-*d*₆ + TFA) δ : 1.48 (d, $J = 6.9$ Hz, 3H), 3.12 (dd, $J = 13.2, 15.5$ Hz, 1H), 3.60 (dd, $J = 2.9, 16.6$ Hz, 1H), 4.60 (d, $J = 11.5$ Hz, 1H), 5.11 (q, $J = 6.9$ Hz, 1H), 6.71 (d, $J = 8.6$ Hz, 1H), 7.15 (d, $J = 8.6$ Hz, 1H), 7.21 (s, 1H), 9.19 (br s, 2H), 9.86 (br s, 1H), 10.97 (br s, 1H). ¹³C-NMR (DMSO-*d*₆ + TFA) δ : 16.9, 29.0, 53.2, 54.5, 107.8, 111.8, 112.0, 114.1, 124.0, 124.4, 131.6, 146.6, 171.9.



Hyrtioreticuline D (4).³

According to the typical procedure for hydrolysis, **4** (17 mg, 70% yield) was obtained as an amorphous white powder.

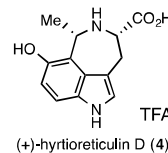
17 mg, 70% yield, an amorphous white powder. $[\alpha]_D^{24} = +14.0$ ($c = 0.55$ in MeOH). Mp: 228-231 °C (CHCl₃/MeOH). IR (CHCl₃): 3447, 1710 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 1.56 (d, $J = 6.9$ Hz, 3H), 3.14 (dd, $J = 13.2, 15.5$ Hz, 1H), 3.39 (dd, $J = 4.0, 16.6$ Hz, 1H), 3.53 (dd, $J = 4.0, 13.2$ Hz, 1H), 5.07 (q, $J = 6.3$ Hz, 1H), 6.65 (d, $J = 9.2$ Hz, 1H), 7.08 (d, $J = 9.2$ Hz, 1H), 7.12 (s, 1H), 8.96 (br s, 1H), 9.01 (br s, 1H), 10.69 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 21.8, 27.8, 50.9, 62.5, 111.0, 112.0, 112.2, 115.0, 123.5, 126.2, 131.6, 146.8, 170.0. HR-ESI-MS m/z : Calcd for C₁₃H₁₅N₂O₃ [(M+H)⁺]: 247.1083. Found 247.1083.



Hyrtioreticuline D (4).

Adding TFA (1 drop) into NMR tube, then ¹H and ¹³C-NMR experiments were performed. Adding TFA (1 μ L) into optical rotation cell, then specific rotation experiment was performed.

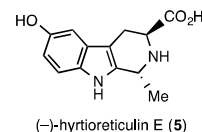
$[\alpha]_D^{24} = +24.0$ ($c = 0.10$ in MeOH-TFA). ¹H-NMR (DMSO-*d*₆ + TFA) δ : 1.62 (d, $J = 7.4$ Hz, 3H), 3.42 (d, $J = 8.1$ Hz, 2H), 4.43 (m, 1H), 5.09 (m, 1H), 6.69 (d, $J = 8.6$ Hz, 1H), 7.13 (d, $J = 8.6$ Hz, 1H), 7.20 (d, $J = 2.3$ Hz, 1H), 8.96 (br s, 1H), 9.58 (br s, 1H), 10.85 (br s, 1H). ¹³C-NMR (DMSO-*d*₆ + TFA) δ : 21.0, 27.5, 52.9, 59.5, 108.5, 112.3, 112.4, 114.0, 124.3, 125.6, 131.5, 147.1, 171.6.



Hyrtioreticulin E (5).¹⁻³

According to the typical procedure for hydrolysis, **5** (23 mg, 93% yield) was obtained as an amorphous white powder.

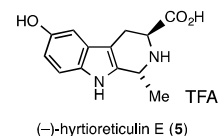
23 mg, 93% yield, an amorphous white powder. $[\alpha]_D^{24} = -47.9$ ($c = 0.11$ in MeOH). Mp: 236–239 °C (CHCl₃/MeOH). IR (CHCl₃): 3446, 1668, 1658 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 1.51 (d, $J = 6.9$ Hz, 3H), 2.82 (dd, $J = 8.0, 15.5$ Hz, 1H), 2.97 (dd, $J = 5.7, 16.1$ Hz, 1H), 3.71 (dd, $J = 5.7, 8.0$ Hz, 1H), 4.55 (q, $J = 6.3$ Hz, 1H), 6.55 (dd, $J = 2.3, 8.6$ Hz, 1H), 6.70 (d, $J = 1.7$ Hz, 1H), 7.06 (d, $J = 8.6$ Hz, 1H), 8.82 (br s, 1H), 10.65 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 18.7, 23.2, 47.2, 53.4, 102.6, 105.2, 112.0, 112.1, 127.3, 131.1, 133.1, 151.1, 170.1. HR-ESI-MS m/z : Calcd for C₁₃H₁₄NaN₂O₃ [(M+Na)⁺]: 269.0902. Found 269.0904.



Hyrtioreticuline E (5).

Adding TFA (1 drop) into NMR tube, then ¹H and ¹³C-NMR experiments were performed. Adding TFA (1 μ L) into optical rotation cell, then specific rotation experiment was performed.

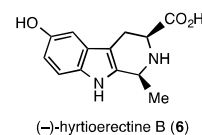
$[\alpha]_D^{24} = -8.8$ ($c = 0.11$ in MeOH-TFA). ¹H-NMR (DMSO-*d*₆ + TFA) δ : 1.61 (d, $J = 6.9$ Hz, 3H), 2.98 (dd, $J = 8.0, 16.0$ Hz, 1H), 3.16 (dd, $J = 5.2, 17.2$ Hz, 1H), 4.55 (t, $J = 6.0$ Hz, 1H), 4.73 (q, $J = 6.9$ Hz, 1H), 6.61 (dd, $J = 2.3, 8.6$ Hz, 1H), 6.74 (d, $J = 2.3$ Hz, 1H), 7.11 (d, $J = 8.6$ Hz, 1H), 9.52 (br s, 1H), 9.80 (br s, 1H), 10.72 (br s, 1H). ¹³C-NMR (DMSO-*d*₆ + TFA) δ : 18.4, 22.4, 47.9, 51.5, 102.7, 103.3, 112.3, 112.6, 126.8, 131.1, 131.8, 151.1, 170.9.



Hyrtiorectine B (6).^{3,4}

According to the typical procedure for hydrolysis, **6** (22 mg, 91% yield) was obtained as an amorphous white powder. Adding TFA (1 μ L) into optical rotation cell, then specific rotation experiment was performed due to its insolubility in MeOH $\{[\alpha]_D^{24} = 0$ ($c = 0.11$ in MeOH)}.

22 mg, 91% yield, an amorphous white powder. $[\alpha]_D^{24} = -69.8$ ($c = 0.11$ in MeOH-TFA). Mp: 264–266 °C (CHCl₃/MeOH). IR (CHCl₃): 3446, 1681 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 1.54 (d, $J = 6.9$ Hz, 3H), 2.66 (m, 1H), 3.01 (dd, $J = 5.2, 16.1$ Hz, 1H), 3.55 (dd, $J = 4.6, 12.0$ Hz, 1H), 4.43 (q, $J = 6.9$ Hz, 1H), 6.56 (dd, $J = 2.3, 8.6$ Hz, 1H), 6.70 (d, $J = 2.3$ Hz, 1H), 7.08 (d, $J = 8.6$ Hz, 1H), 8.78 (br s, 1H), 10.75 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 17.4, 23.8, 49.7, 58.2, 102.6, 106.4, 112.0, 112.1, 127.3, 131.3, 132.9, 151.2, 170.0. HR-ESI-MS m/z : Calcd for C₁₃H₁₄NaN₂O₃ [(M+Na)⁺]: 269.0902. Found 269.0900.



References

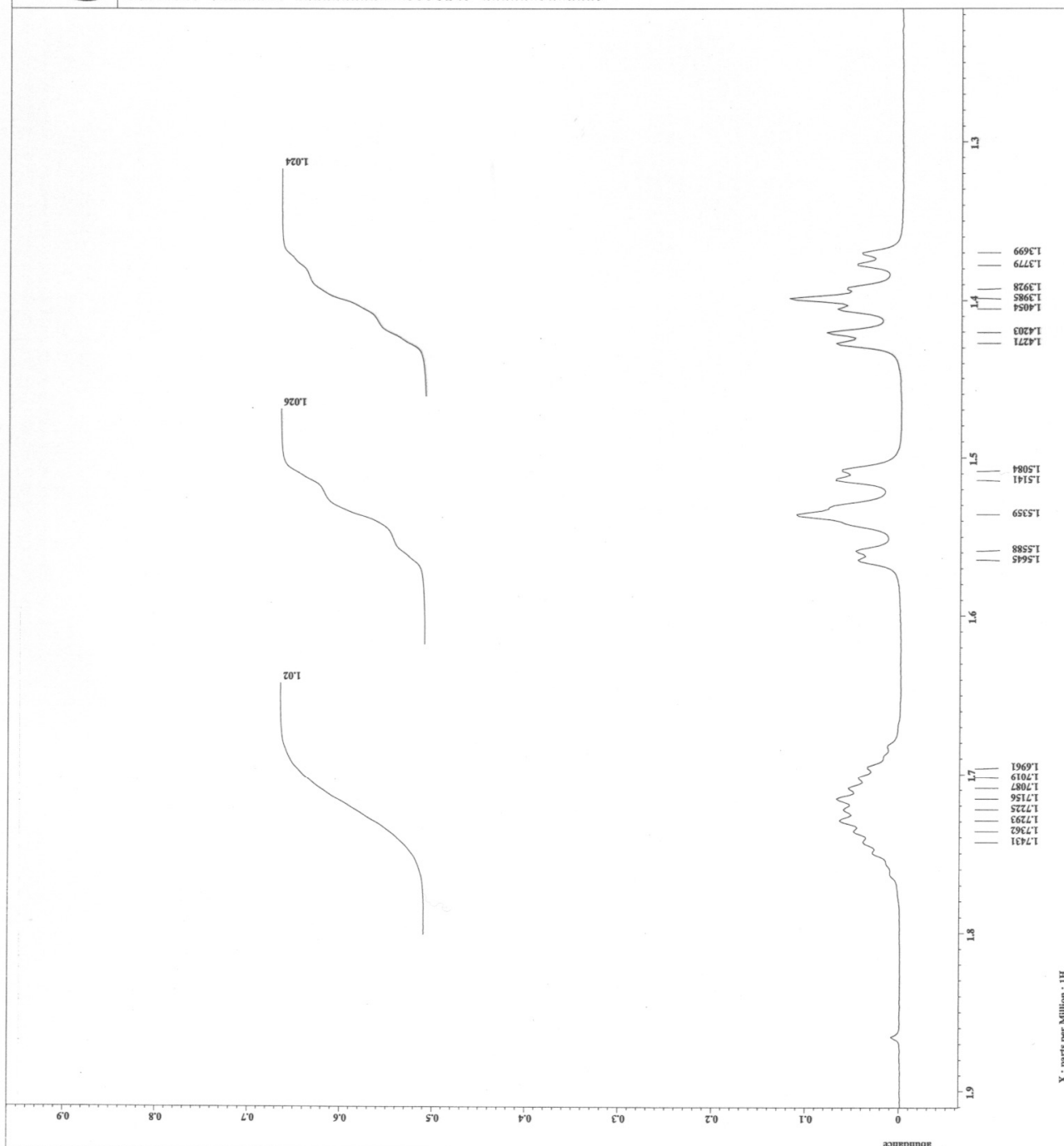
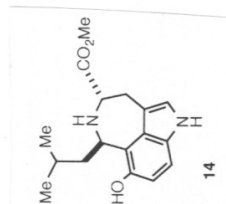
- (1) Brossi, A.; Focella, A.; Teitel, S. *J. Med. Chem.* **1973**, *16*, 418–420.
- (2) Teital, S.; Brossi, A. *Lloydia* **1974**, *37*, 196–211.
- (3) Yamanokuchi, R.; Imada, K.; Miyazaki, M.; Kato, H.; Watanabe, T.; Fujimuro, M.; Saeki, Y.; Yoshinaga, S.; Terasawa, H.; Iwasaki, N.; Rotinsulu, H.; Losung, F.; Mangindaan, R. E. P.; Namikoshi, M.; de Voogd, N. J.; Yokosawa, H.; Tsukamoto, S. *Bioorg. Med. Chem.* **2012**, *20*, 4437–4442.
- (4) Youssef, D. T. A. *J. Nat. Prod.* **2005**, *68*, 1416–1419.



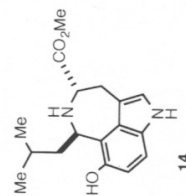
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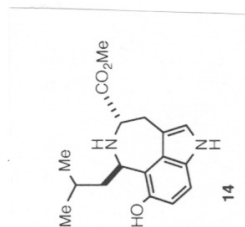
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Experiment     = single_pulse.exe
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Revision_time  = 15-DEC-2016 13:56:07
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Dir_units      = [ppm]
Dir_extensions =
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X_points       = 512
X_resolution   = 16384
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X_tr_offset    = 5[ppm]
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X_tr_offset    = 5[ppm]
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X_tr_offset    = 64
Total_scans    = 64
X_90_width     = 12.7[us]
X_acq_time     = 1.76422912[s]
X_angle        = 45[deg]
X_tr_delay     = 6.31[us]
X_pulse        = Off[us]
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X_tr_delay     = 1[s]
Initial_wait   = 36
Rever_gain     = 36
Rever_delay    = 6.76422912[s]
Repetition_time = 20.4[sec]
Temp_get       =
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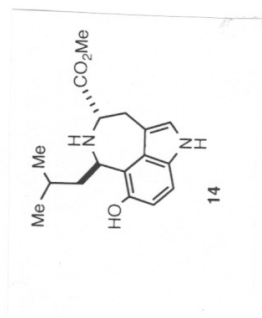
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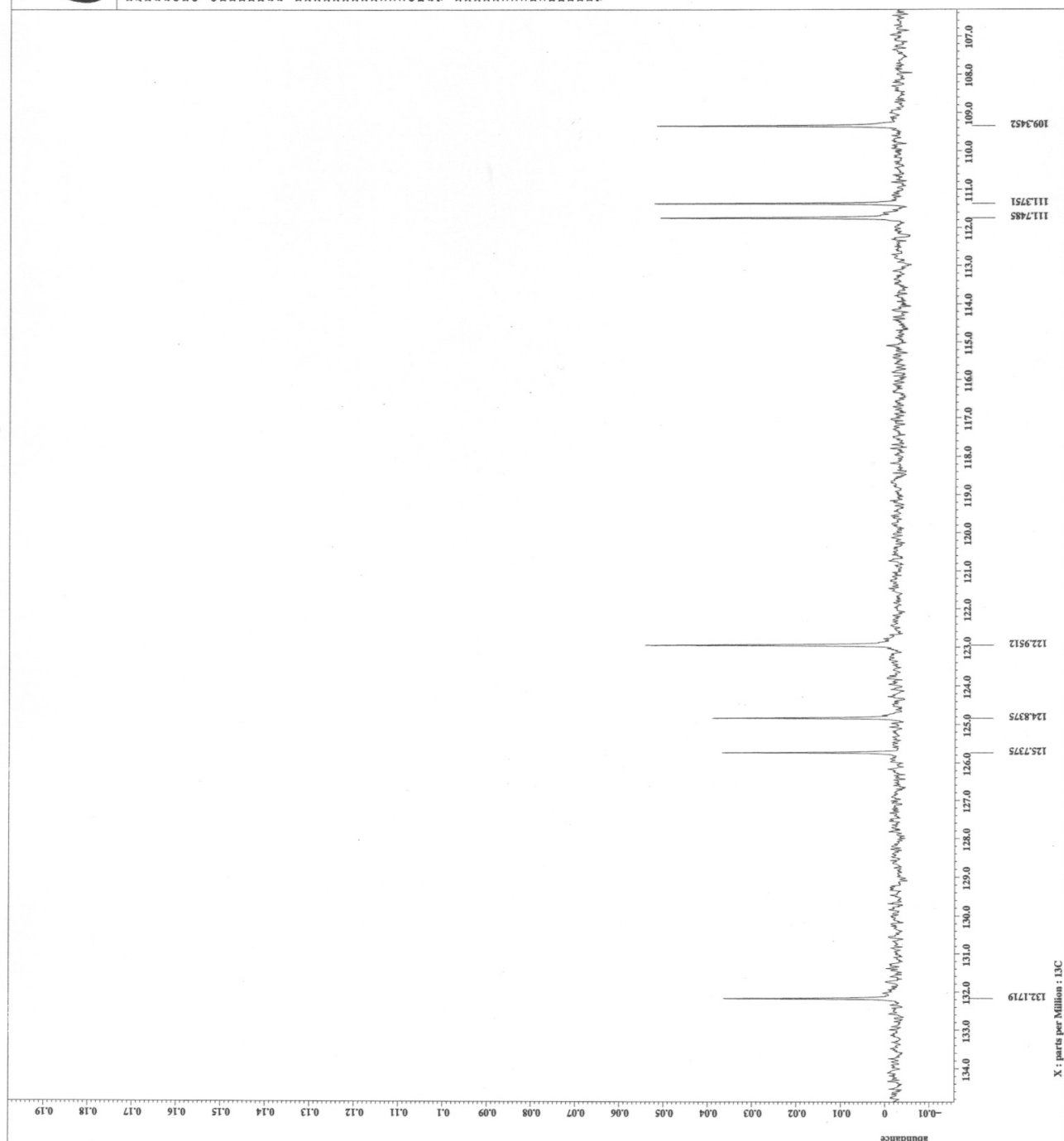
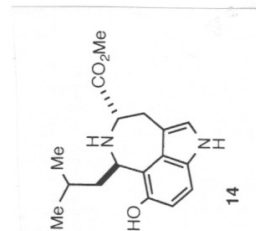


X : parts per Million : 1H

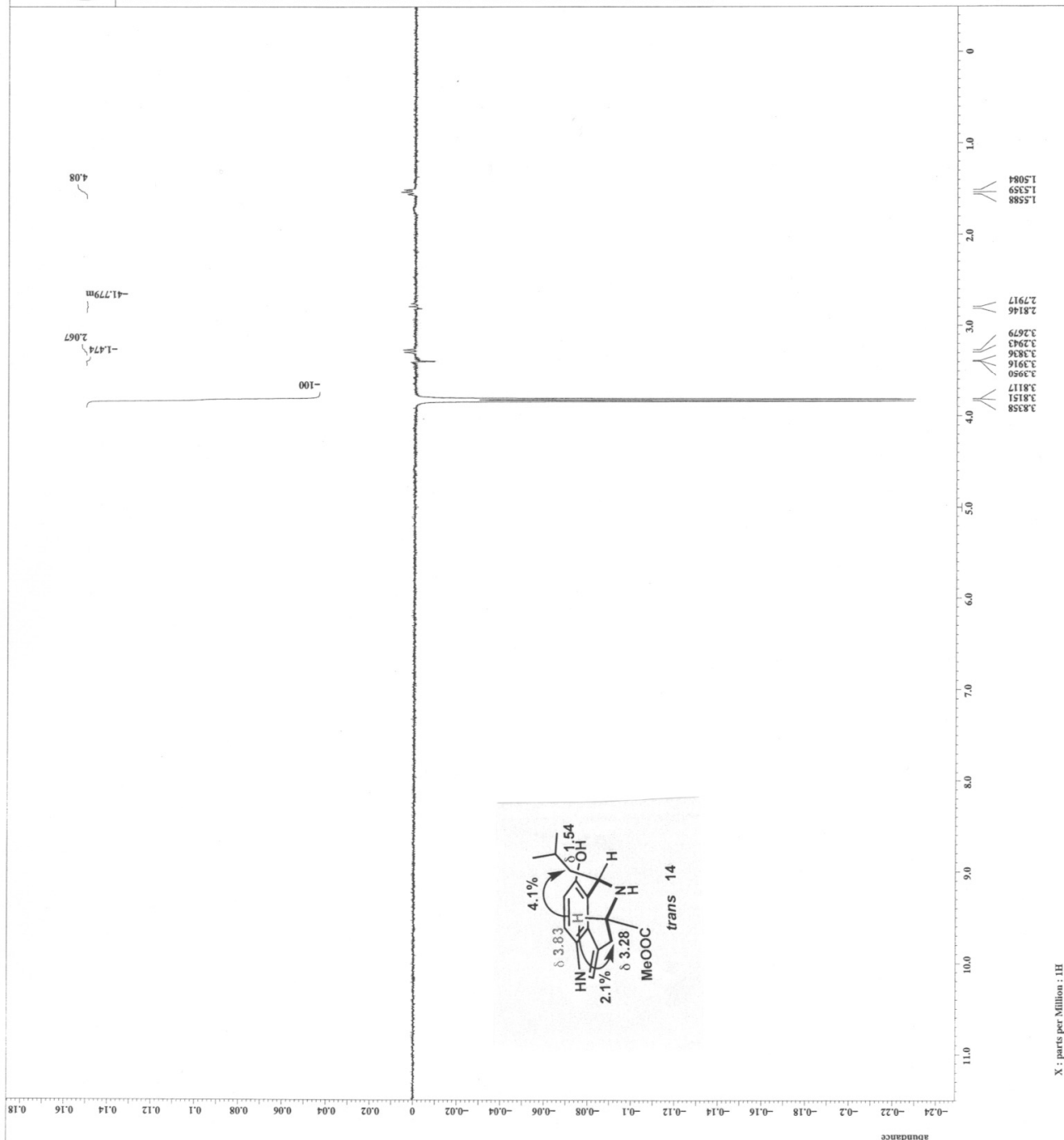






[illegible]





```

----- PROCESSING PARAMETERS
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ppm
Derived from: yama-16-12-10-11.jdr

```

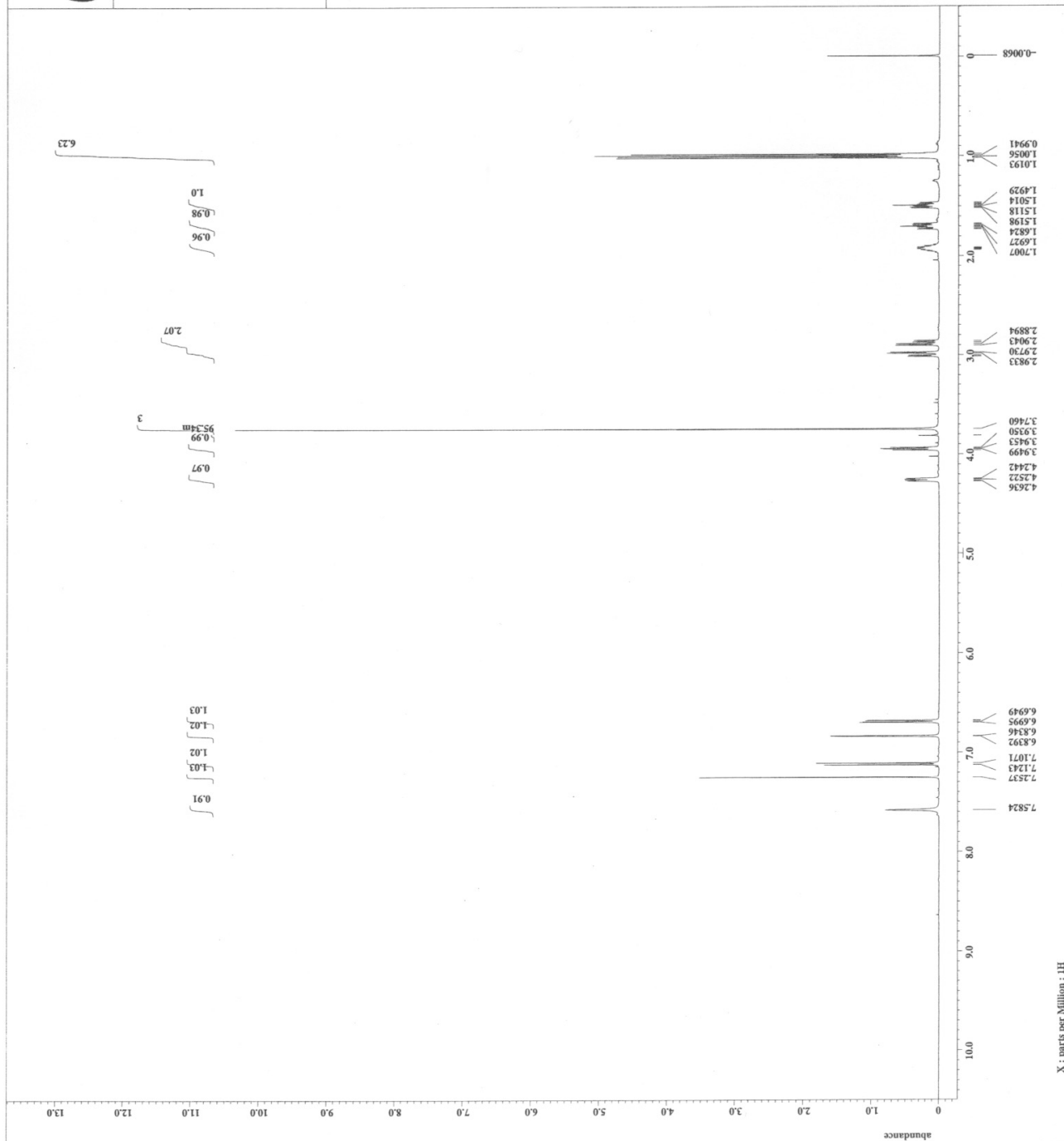
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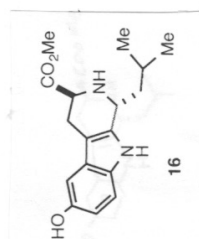
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Author        =
Experiment     = S18F873_pulse_exs2
Solvent        = CHLOROFORM-D
Creation_time  = 11-DEC-2016 09:12:09
Curation_time = 11-DEC-2016 10:12:09
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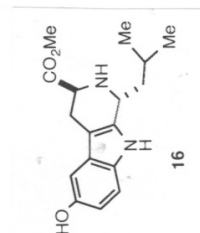
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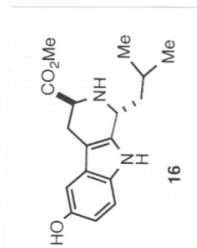
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X : parts per Million : 1H



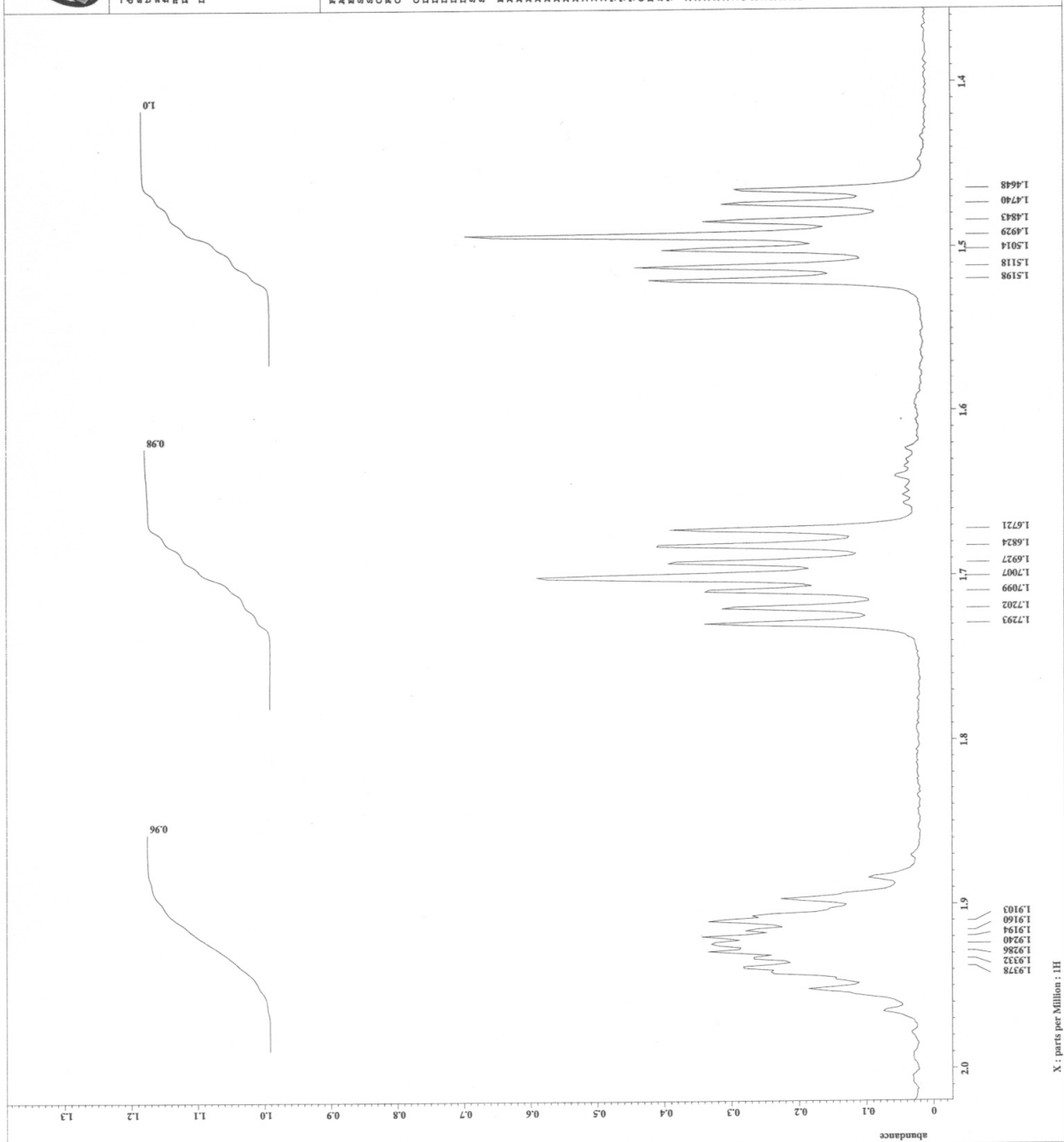
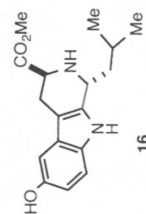


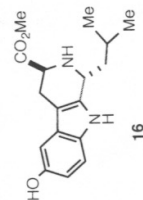




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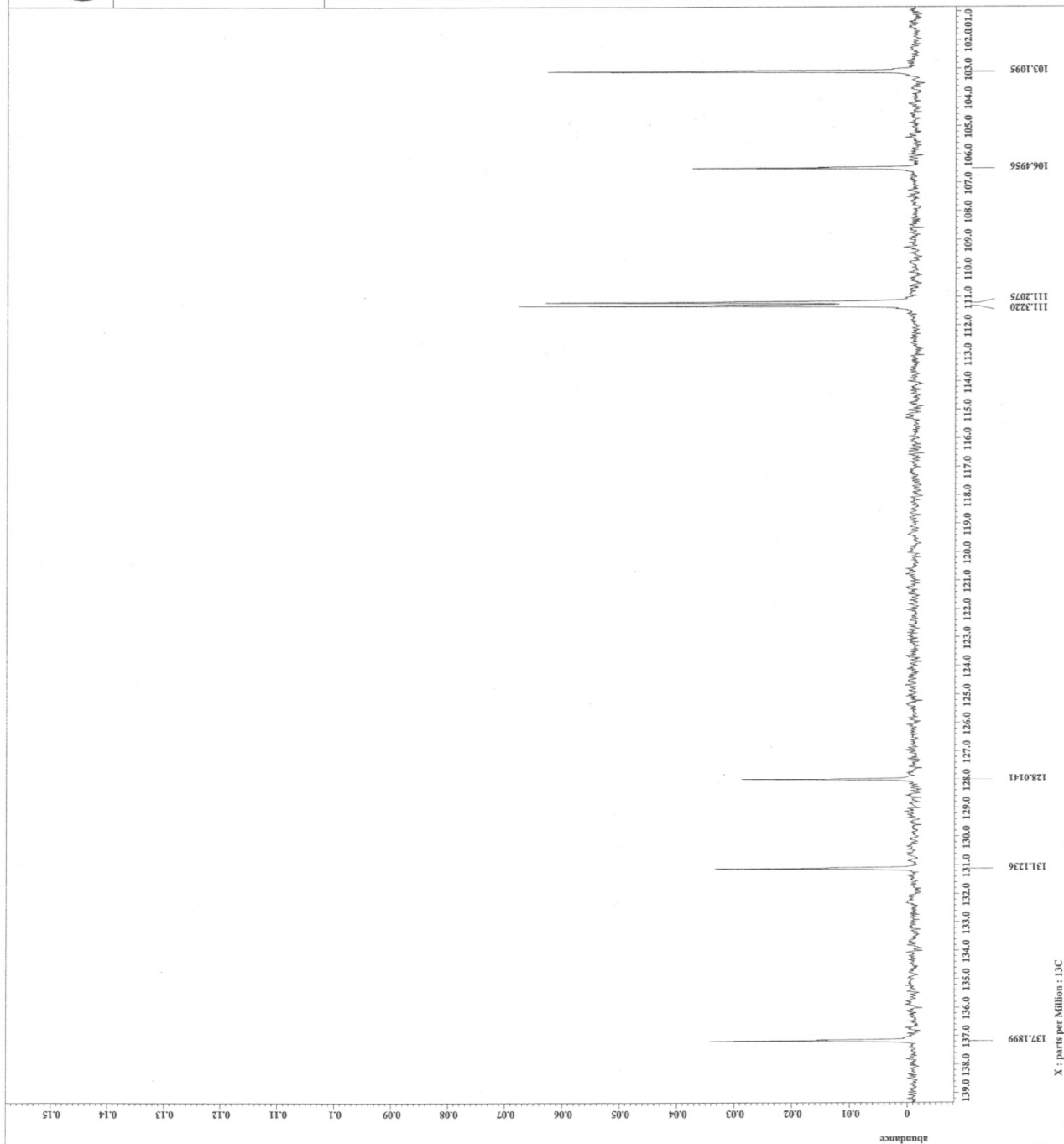
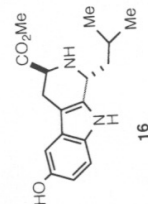
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X_freq = 500.1321 [MHz]
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X_sweep = 9.38438438 [MHz]
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Data_return = 1
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X_acq_time = 1.74387904 [s]
X_angle = 4.5 [deg]
X_p1 = 5.0 [us]
X_p2 = 5.9 [us]
Irr_p1 = OFF
Irr_p2 = OFF
Data_preset = FALSE
Initial_wait = 1 [s]
Acquire_delay = 5.0 [s]
Relaxation_delay = 5 [s]
Repetition_time = 6.74387904 [s]
Temp_get = 22.4 [degC]





--- PROCESSING PARAMETERS ---
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 traspcid4 : 0 [%] : 80 [%] : 100 [%]
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 ppm
 Derived from: yama-16-12-10-12-jdf

File name : yama-16-12-10-14-jdf
 Author :
 Experiment :
 Sample_id :
 Solvent : CHLOROFORM-D
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 Revision_time : 12-DEC-2016 07:10:55
 Current_time : 12-DEC-2016 07:12:14
 Comment :
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 Dia_time :
 Dia_title :
 Dia_file :
 Dimensions :
 Site :
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 X_acq_time : 0.83362792 [s]
 X_freq : 125.76529768 [MHz]
 X_offset : 10.0 [ppm]
 X_resolution : 4
 X_resolution : 1.19959034 [Hz]
 X_sweep : 39.3081761 [MHz]
 X_freq : 500.15991521 [MHz]
 X_offset : 5.0 [ppm]
 X_pulse : 1
 Mod_return : 26496
 Total_scans : 26496
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 X_delay : 5.5 [s]
 X_atn : 5.5 [dB]
 X_pulse_dec : 3.7666667 [us]
 X_acq_time : 21.238 [s]
 X_atn_dec : 21.238 [dB]
 X_noise : VALTZ
 Decoupling : 1
 Modulation : 1
 Noe : TRUE
 Noe_time : 2 [s]
 Relaxation_delay : 2 [s]
 Repetition_time : 2.83362792 [s]
 Temp_get : 23.3 [C]



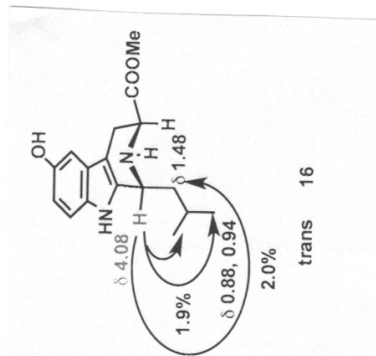


--- PROCESSING PARAMETERS ---
ac balance 0 : FALSE
sweep 0 : 0.2[Hz] : 0.0[s]
xresol 0.3 : 0[N] : 80[N] : 100[N]
fft 1 : TRUE : TRUE
ppm
Phase : 164 : 0 : 50[N]
Derived from: yama-16-12-20-trans-3.jdr

Filename = yama-16-12-20-trans-1
Filepath =
Experiment = noe_1d_dpfgae.ex
Sample_id = yama
Acq_date = 20-DEC-2016 18:13:52
Creation_time = 21-DEC-2016 07:35:42
Revision_time = 21-DEC-2016 07:35:50
Current_time =
Comment = DFGSE NOE 1d
Data_format = 1D COMPLEX
F2_id = 11.07
Dim_title = [ppm]
Dim_units = [ppm]
Dimensions = 2
Spectrometer = DELTA2_MMR
Field_strength = 11.7413579[G] (500[MH]
X_acq_duration = 1.74567904[s]
X_domain = 1H
X_freq = 500.13991521[MHz]
X_offset = 0.00000000[ppm]
X_points = 16384
X_resolution = 2.5727737[Hz]
X_sweep = 9.38438436[MHz]
X_center = 500.13991521[MHz]
Irr_domain = 1H
Irr_freq = 500.13991521[MHz]
Irr_offset = 0.00000000[ppm]
Tri_domain = 1H
Tri_freq = 500.13991521[MHz]
Tri_offset = 0.00000000[ppm]
Clipped = FALSE
Mod_return = 1
Gain = 1648
TOTAL_scans = 2048
X_acq_time = 1.74567904[s]
X_pulse = 11.8[us]
Irr_mode = Off
Obs_sol = 80
Obs_sol_atn = 54.23[dB]
Obs_sol_offset = 4.0238[ppm]
Obs_sol_shape = G0089
Obs_sol_sfp = 0.00000000[ppm]
Tri_mode = Off
Data_preset = FALSE
Grat_1_amp = 60[mV/m]
Grat_1_freq = 1[Hz]
Grat_2_amp = 10[mV/m]
Grat_2_freq = 30[mV/m]
Grat_3_amp = 0.1[Hz]
Grat_3_freq = 0.1[Hz]
Grat_recover = 1[s]
Initial_wait = 1[s]
Mix_time = 0.5[s]
Rever_gain = 7.0
Rever_gain_delay = 7.0
Repetition_time = 8.74567904[s]
Temp_get = 22.4[degC]

1.93
2.0
0.52
1.88
0.49
75.88mm

-100



0.8773
0.9133
0.9323
0.9449
1.4602
1.4751
1.4900
1.5037
1.8553
1.8691
1.8828
2.5951
3.3005
3.6006
4.0243
4.0701
4.0827
4.0976
5.0
6.0
7.0
8.0
9.0
10.0
11.0

X : parts per Million : 1H

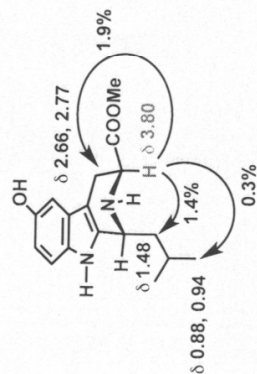


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 mag : 0.2 [Hz], 0.0 [s]
 zascfill : 1
 f1 : 1 : TRUE : TRUE
 phase : 164 : 0 : 50 [%]
 Derived from: yama-16-12-20-trans-5.jcf

Filename = yama-16-12-20-trans-9
 Author = Delta
 Experiment = nmr_id_obfgee.ex
 Name = DMSO-D6
 Solvent = DMSO-D6
 Creation_time = 20-DEC-2016 23:31:22
 Start_time = 20-DEC-2016 23:31:22
 Current_time = 21-DEC-2016 07:31:37
 Comment = NMR of trans-16
 Data_dir = 1107
 Dim_size = 1H
 Dimensions = 1 (ppm)
 Site = ECA500
 Spectrometer = DELTA 500
 Field_strength = 11.7473579 [T] (500 [MHz])
 X_acq_duration = 1.74587904 [s]
 X_acq_time = 1.74587904 [s]
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_resolution = 2.6384
 X_resolution = 0.5277737 [Hz]
 X_sweep = 9.38438438 [kHz]
 X_center = 500.15991521 [MHz]
 X1_freq = 5.0 [ppm]
 X2_freq = 500.15991521 [MHz]
 X1_offset = FALSE
 X2_offset = FALSE
 Clipped = FALSE
 Scans = 2048
 Total_scans = 2048
 X_acq_time = 1.74587904 [s]
 X_atn = 3.4 [dB]
 X_pulse = 21.0 [us]
 Obs_sel_180 = 20 [ms]
 Obs_sel_atn = 54.235 [dB]
 Obs_sel_offset = 3.7976 [ppm]
 Obs_sel_phase = 3.7976 [ppm]
 Tri_mode = Off
 Grad1_presat = 1 [ms]
 Grad1_amp = 60 [Hz/m]
 Grad2_presat = 1 [ms]
 Grad2_amp = 90 [Hz/m]
 Grad3_presat = 1 [ms]
 Grad3_amp = 30 [Hz/m]
 Grad4_presat = 1 [ms]
 Grad4_amp = 30 [Hz/m]
 Grad_shape = SINC
 Initial_wait = 1 [s]
 Mix_time = 5.0 [s]
 Relaxation_delay = 7 [s]
 Repetition_time = 8.74587904 [s]
 Temp_set = 22.4 [C]

0.16 0.23 0.31 2.88 0.19 1.39 0.34

100



trans 16

4.0833 3.8079 3.7850 3.6750 3.6006 3.4517 3.3005 2.7760 2.7451 2.6684 2.6409 1.8805 1.8679 1.5037 1.4900 1.4763 1.4591 0.9449 0.8922 0.8785

X : parts per Million : 1H

```
dc_balance : 0 : FALSE
semp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
zfc : 1 : TRUE : TRUE
ppm
phase : -196 : 0 : 50[%]
```

Derived from: yama-16-12-20-trans-5.jdf

```

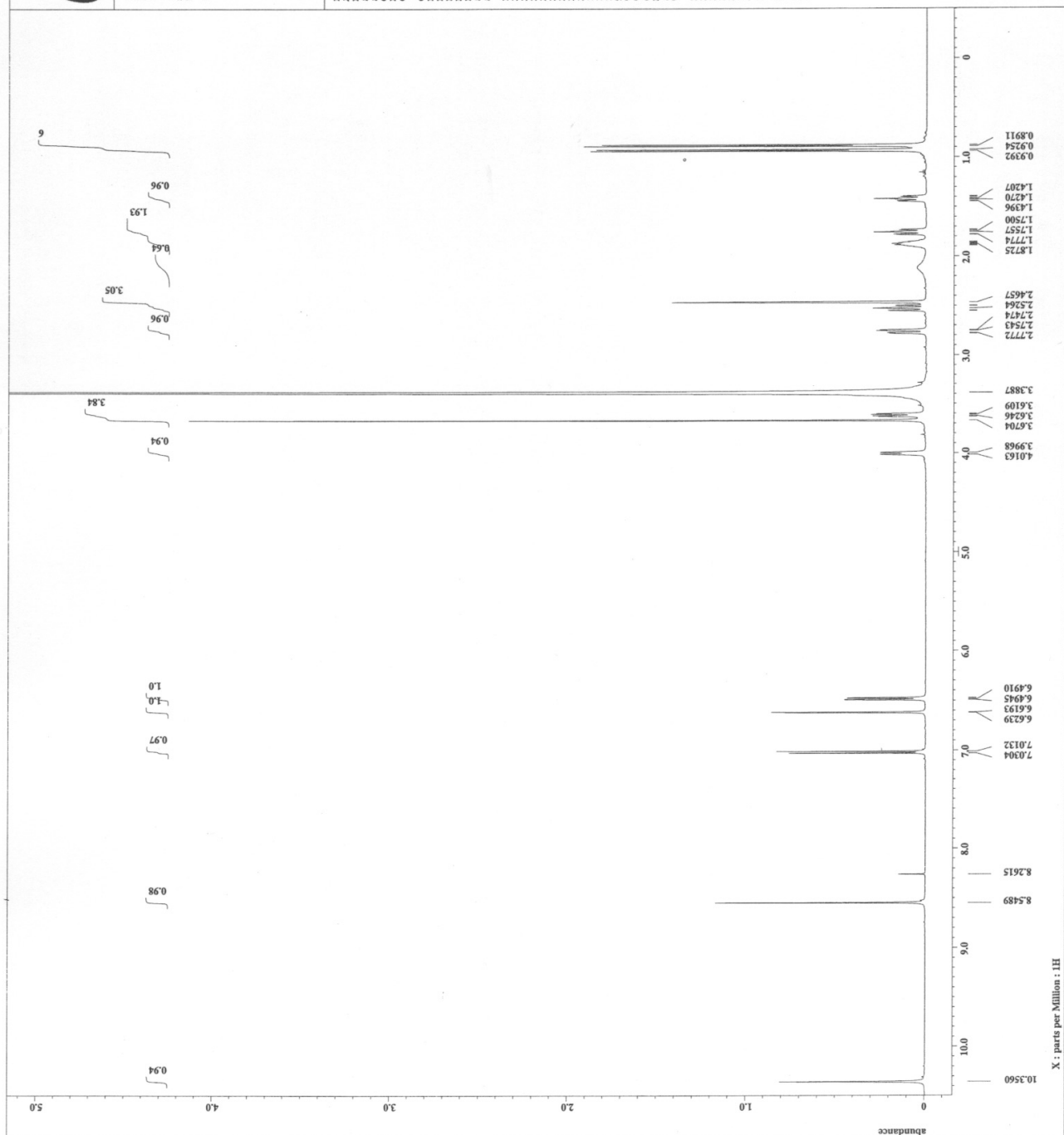
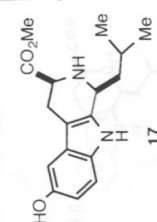
# Yema-16-12-20-trans=
# Data
# no_id_offset.exe
# Yema-D6
# 20-DEC-2016 23:31:22
# 21-DEC-2016 13:50:49
# 22-DEC-2016 13:50:49
# DPGFOS NOE ID
# 13107
# 1K
# [ppm]
# KAI500
# DELTA_MNR
# 11.7473579(4) (500) MHz
# 1.74587904(s)
# 130.15894521[MHz]
# 5.0[ppm]
# 16384
# 0.52727737[Hz]
# 9.38438843[MHz]
# 18.15894521[MHz]
# 5.0[ppm]
# 1K
# 500.15894521[MHz]
# FALSE
# 1.646
# 2648
# 1.74587904(s)
# 11.8[sus]
# Off
# Off
# 5.231[D3]
# 3.7976[ppm]
# GAUSS
# 0.52727737[ppm]
# Off
# FALSE
# 1[sus]/m
# 1[sus]/m
# 90[deg/m]
# 30[deg/m]
# 0.1[sus]
# SINE
# Mix time = 0.5[s]
# 50
# Recv_gain
# Relaxation delay = 1.74587904[s]
# 22.4[s]
# Time_per

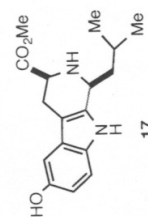
```





Derived from: yama-16-12-12-1.1ddf

[illegible]



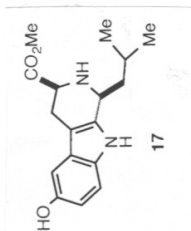
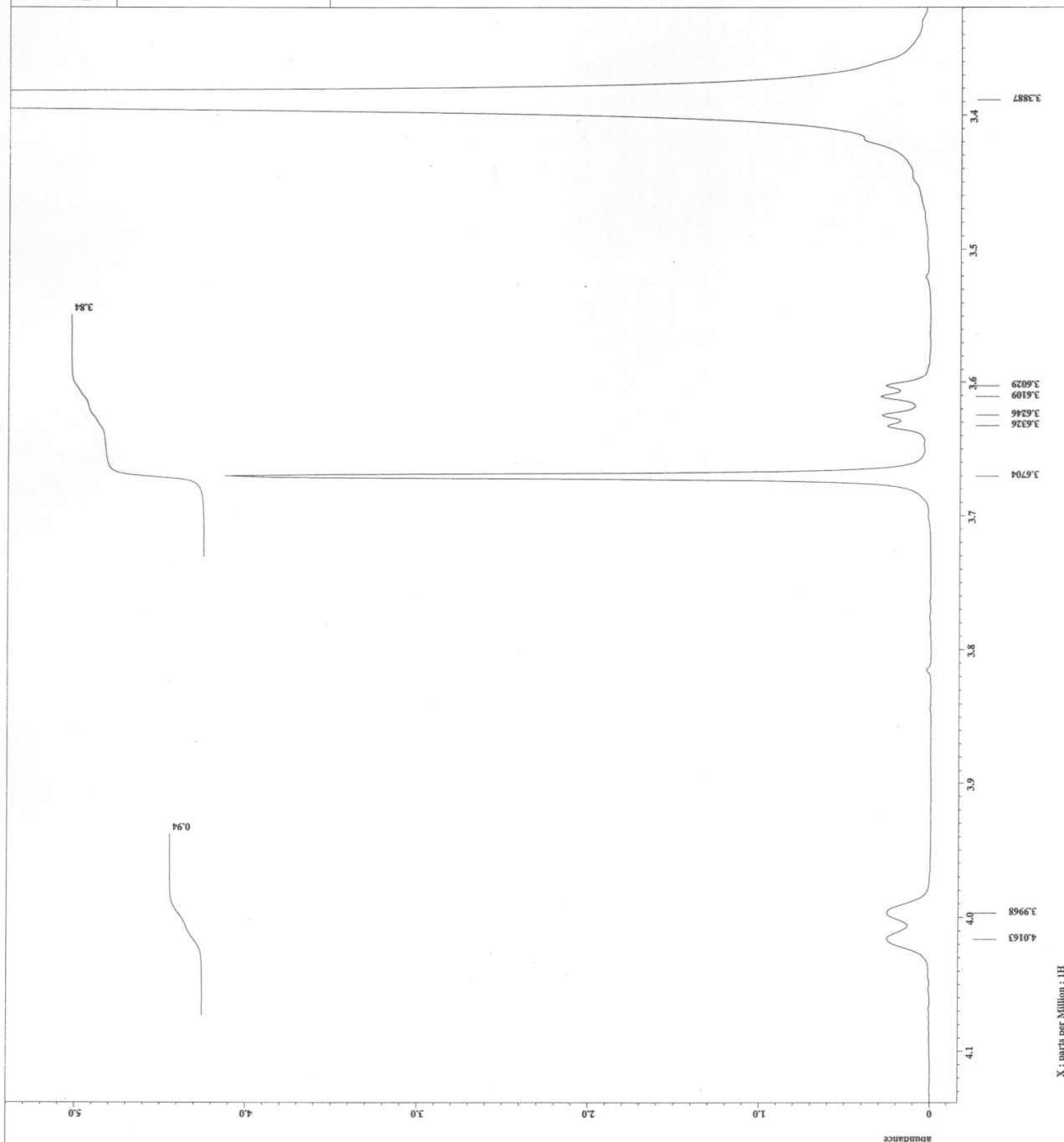
----- PROCESSING PARAMETERS -----

```

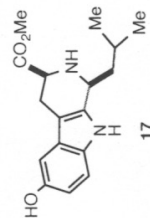
dc balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm

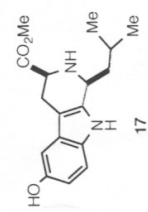
```

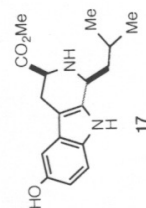
Derived from: yama-16-12-12-1-1.jdf



X : parts per Million : 1H







X : parts per Million : 13C

Derived from: yama-16-12-12-2.jdf

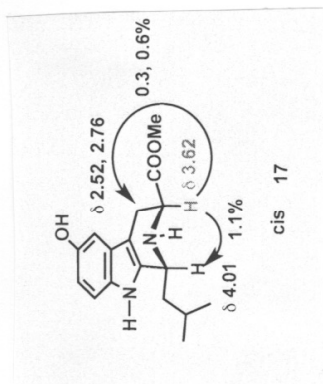
```
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 23.6[dc]
```



Filename = yama-16-12-20-cis-10.
 Author = delta
 Experiment = noe_1d_dpfgmh.ex
 Solvent = DMSO-D6
 Creation_time = 21-DEC-2016 04:40:15
 Acquisition_time = 21-DEC-2016 07:17:13
 Current_time = 21-DEC-2016 07:17:13
 Content = DPFGSE NOE 1d
 ID = 13107
 ID COMPACT = 13107
 IN = 1H
 X = 13C
 Dimensions = ECA 500
 Site = DELTA2_NMR
 Spectrometer =
 Field_strength = 11.6226421[T] (500[M
 X_acq_duration = 1.76422912[s]
 X_freq = 495.13191398[MHz]
 X_offset = 5[ppm]
 X_resolution = 0.5668198[Mz]
 X_resolution_h = 0.5668198[Mz]
 X_resolution_v = 0.5668198[Mz]
 Irr_freq = 495.13191398[MHz]
 Irr_offset = 5[ppm]
 Tri_freq = 495.13191398[MHz]
 Tri_offset = 5[ppm]
 Mod_return = 1
 Scans = 2048
 Total_scans = 2048
 X_acq_time = 1.76422912[s]
 X_atn = 1.0[DB]
 X_f1 = 100
 Irr_mode = OFF
 Obs_sel_180 = 20[ms]
 Obs_sel_offset = 3.6125[ppm]
 Obs_sel_shape = GAUSS
 Obs_sel_alp = 0.125[ppm]
 Tri_mod = FALSE
 Data_preset = 1[ms]
 Grad_1 = 1[ms]
 Grad_2 = 30[ms]
 Grad_3 = 1[ms]
 Grad_4 = 10[ms]
 Grad_5 = 10[ms]
 Grad_recovery = 0.1[ms]
 Grad_shape = 1[ms]
 Grad_shape2 = 1[ms]
 Mix_time = 0.5[s]
 Recvr_gain_delay = 50
 Repetition_time = 8.76422912[s]
 Temp_get = 22.1[OC]

0.276
0.63
0.796
1.13

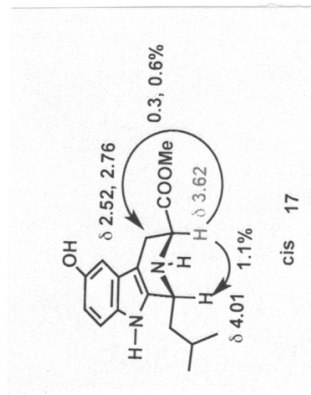
-100
-132.51



abundance

2.4998
2.5192
2.5284
2.7459
2.7757
3.6045
3.6263
3.6343
3.6698
3.6972
4.0155

X : parts per Million : 1H



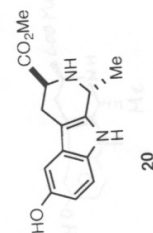
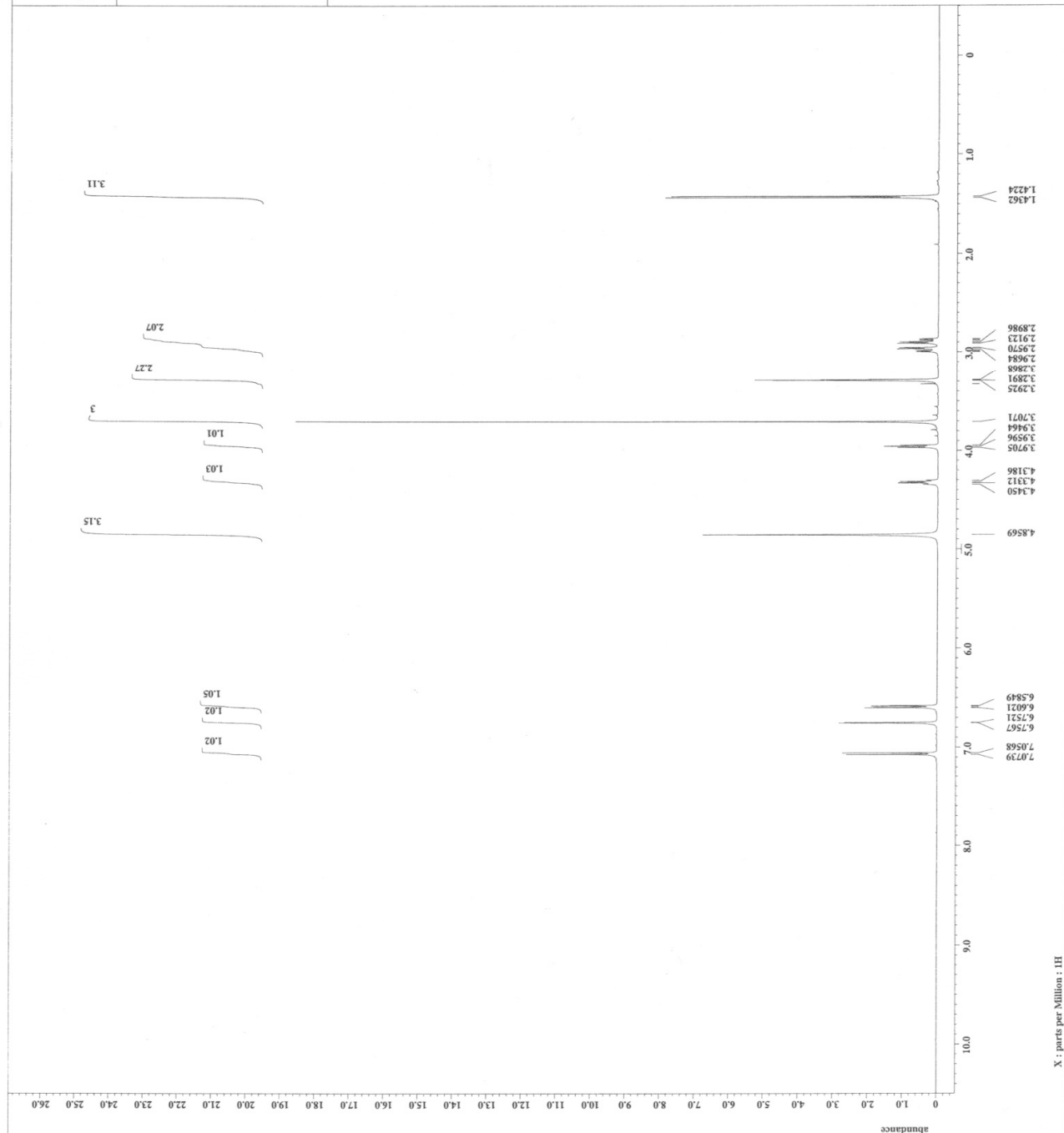
Filepath	= data
Experiment	= nos
Experiment	= nos
Solvent	= DMF5-D6
Creation_time	= 21-MAR-2016 10:40:15
Creation_time	= 21-MAR-2016 10:40:15
Current_time	= 21-MAR-2016 07:42:07
Content	= DPFGSE NOE 1d
Content	= DPFGSE NOE 1d
Dia_size	= 13107
Dia_title	= 1H
Dia_unit	= [ppm]
Dia_dimensions	= ECA 500
Site	= DELTA2_MMR
Spectrometer	= 1H_12926421[7] (500IM
Flt_strength	= 1.764229212[s]
X_acq_duration	= 1.764229212[s]
X_domain	= 135.13193398 [kHz]
X_offset	= 5 [ppm]
X_pos	= 16394
X_resolution	= 0.5668198 [Hz]
X_swap	= 9.2667563 [kHz]
Yir_domain	= 135.13193398 [kHz]
Yir_offset	= 5 [ppm]
Yir_domain	= 1H
Yir_freq	= 499.13193398 [MHz]
Yir_offset	= FALSE
Yir_clip	= 1
Yir_return	= FALSE
Total_scans	= 2048
X_acq_time	= 1.764229212[s]
X_pulse	= 13.7 [us]
Xir_mode	= OFF
Obs_sel_160	= 5 [ppm]
Obs_sel_160	= 5 [ppm]
Obs_sel_offset	= 3.6125 [ppm]
Obs_sel_shape	= GAUSS
Obs_sel_amp	= 0.125 [ppm]
Obs_sel_pos	= FALSE
Dantc_preset	= 1 [ms]
Grad_1_amp	= 1 [ms]
Grad_2_amp	= 1 [ms]
Grad_3_amp	= 30 [us]
Grad_4_amp	= 1 [ms]
Grad_5_amp	= 1 [ms]
Grad_recovery	= 0.1 [ms]
Grad_shape	= SINE
Grad_pos	= 0.1 [ms]
Grad_wait	= 0.1 [ms]
MX_time	= 50
Recvr_gain	= 75 [dB]
Relaxation_delay	= 21.1565 [s]
Relaxation_time	= 22.1565 [s]
Post_get	= 22.1565 [s]

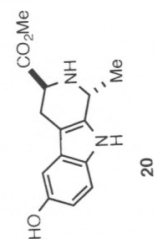
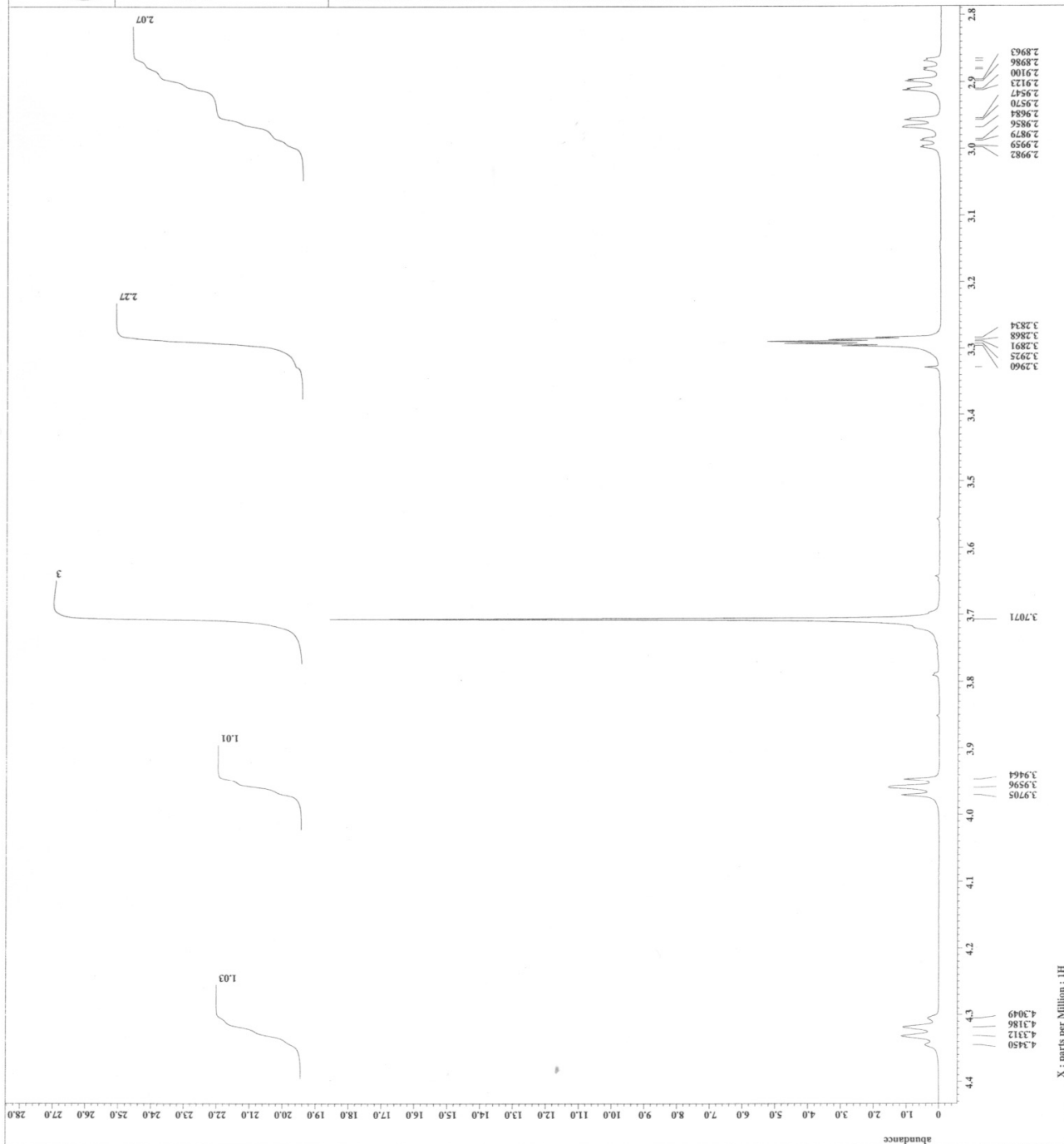
```

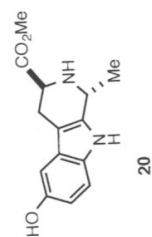
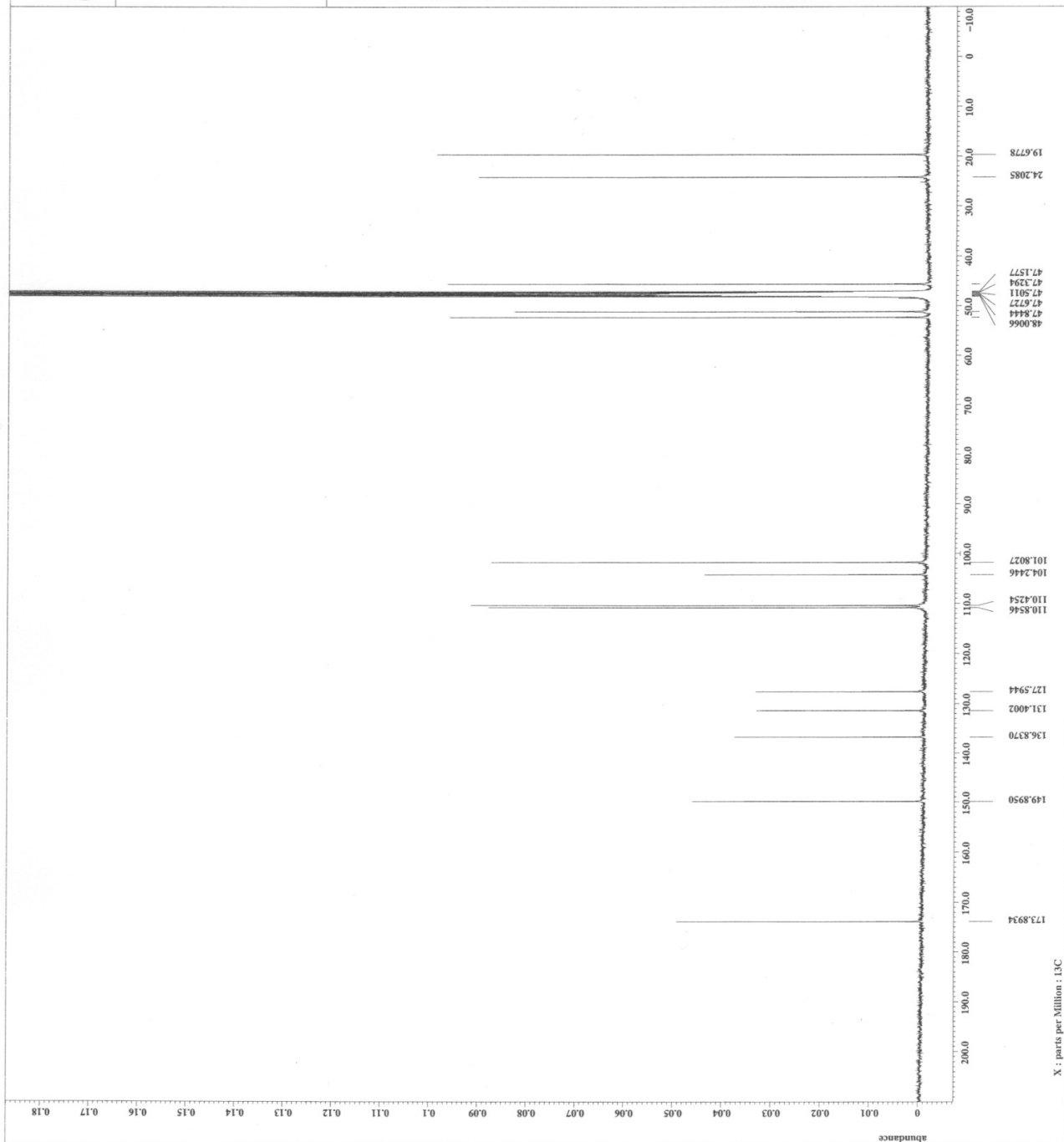
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
semp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
Derived from: yama-16-12-09-1.jde

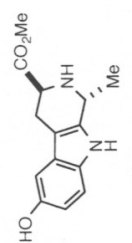
```

Derived from: yama-16-12-09-1.1.jdf

[illegible]







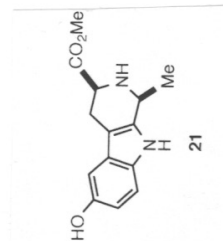

```

----- PROCESSING PARAMETERS -----
dc bal 0.3 [Hz] : 0 %
sorp : 0.3 [Hz] : 0 %
trapzoid1 : 0 % : 80 % : 100 %
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from:Hydrorectine B Me-ester-

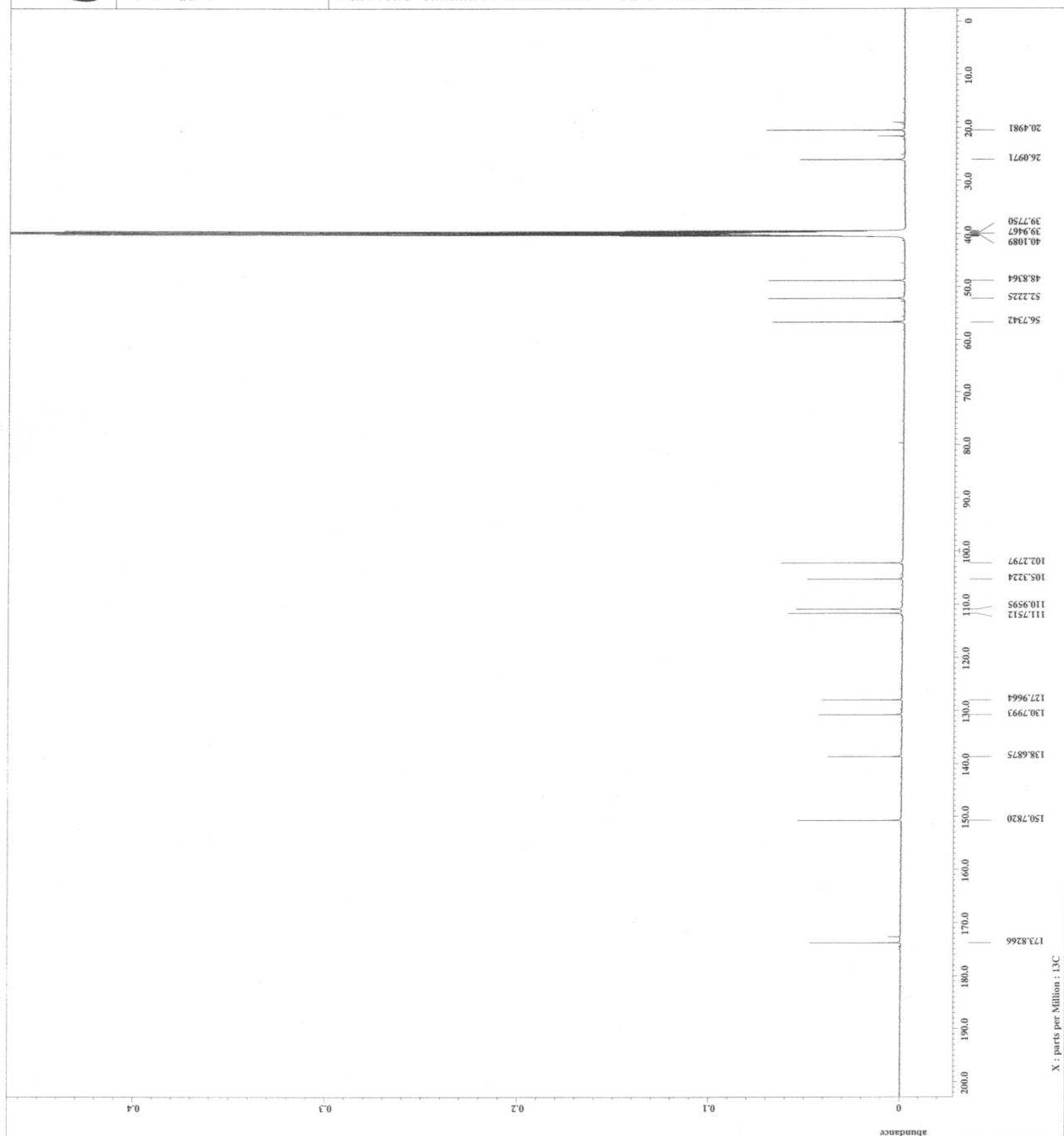
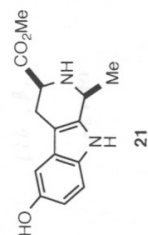
```

Derived from: Hyrtioerectine B Me-ester-

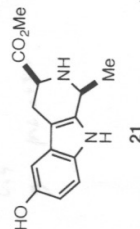
Filename	ByteIOStream3_Memo
Author	Gatta
Experiment	EMSA_Pulse.exe2
Sample	EMSA-D5
Solvent	DMSO-d6
Creation_time	2-DEC-2016 12:11:35
Creation_date	2-DEC-2016 12:11:35
Current_time	2-DEC-2016 17:58:28
Current_date	2-DEC-2016 17:58:28
Comment	EMSA-D5_NMR
Container	EMSA-D5_NMR
Container_type	EMSA-D5_NMR
Container_size	11.7473579 [s] (500 [Hz]
Container_resolution	11.747357904 [s]
Container_x_resolution	11.747357904 [s]
Container_y_resolution	11.747357904 [s]
Container_z_resolution	11.747357904 [s]
Container_x_max	50.155991521 [Hz]
Container_y_max	50.155991521 [Hz]
Container_z_max	50.155991521 [Hz]
Container_x_min	50.155991521 [Hz]
Container_y_min	50.155991521 [Hz]
Container_z_min	50.155991521 [Hz]
Container_x_center	50.155991521 [Hz]
Container_y_center	50.155991521 [Hz]
Container_z_center	50.155991521 [Hz]
Container_x_delta	50.155991521 [Hz]
Container_y_delta	50.155991521 [Hz]
Container_z_delta	50.155991521 [Hz]
Container_x_stddev	50.155991521 [Hz]
Container_y_stddev	50.155991521 [Hz]
Container_z_stddev	50.155991521 [Hz]
Container_x_rms	50.155991521 [Hz]
Container_y_rms	50.155991521 [Hz]
Container_z_rms	50.155991521 [Hz]
Container_x_mean	50.155991521 [Hz]
Container_y_mean	50.155991521 [Hz]
Container_z_mean	50.155991521 [Hz]
Container_x_std	50.155991521 [Hz]
Container_y_std	50.155991521 [Hz]
Container_z_std	50.155991521 [Hz]
Container_x_rmsd	50.155991521 [Hz]
Container_y_rmsd	50.155991521 [Hz]
Container_z_rmsd	50.155991521 [Hz]
Container_x_rmsd_max	50.155991521 [Hz]
Container_y_rmsd_max	50.155991521 [Hz]
Container_z_rmsd_max	50.155991521 [Hz]
Container_x_rmsd_min	50.155991521 [Hz]
Container_y_rmsd_min	50.155991521 [Hz]
Container_z_rmsd_min	50.155991521 [Hz]
Container_x_rmsd_center	50.155991521 [Hz]
Container_y_rmsd_center	50.155991521 [Hz]
Container_z_rmsd_center	50.155991521 [Hz]
Container_x_rmsd_delta	50.155991521 [Hz]
Container_y_rmsd_delta	50.155991521 [Hz]
Container_z_rmsd_delta	50.155991521 [Hz]
Container_x_rmsd_stddev	50.155991521 [Hz]
Container_y_rmsd_stddev	50.155991521 [Hz]
Container_z_rmsd_stddev	50.155991521 [Hz]
Container_x_rmsd_rms	50.155991521 [Hz]
Container_y_rmsd_rms	50.155991521 [Hz]
Container_z_rmsd_rms	50.155991521 [Hz]
Container_x_rmsd_mean	50.155991521 [Hz]
Container_y_rmsd_mean	50.155991521 [Hz]
Container_z_rmsd_mean	50.155991521 [Hz]
Container_x_rmsd_std	50.155991521 [Hz]
Container_y_rmsd_std	50.155991521 [Hz]
Container_z_rmsd_std	50.155991521 [Hz]
Container_x_rmsd_rmsd	50.155991521 [Hz]
Container_y_rmsd_rmsd	50.155991521 [Hz]
Container_z_rmsd_rmsd	50.155991521 [Hz]
Container_x_rmsd_rmsd_max	50.155991521 [Hz]
Container_y_rmsd_rmsd_max	50.155991521 [Hz]
Container_z_rmsd_rmsd_max	50.155991521 [Hz]
Container_x_rmsd_rmsd_min	50.155991521 [Hz]
Container_y_rmsd_rmsd_min	50.155991521 [Hz]
Container_z_rmsd_rmsd_min	50.155991521 [Hz]
Container_x_rmsd_rmsd_center	50.155991521 [Hz]
Container_y_rmsd_rmsd_center	50.155991521 [Hz]
Container_z_rmsd_rmsd_center	50.155991521 [Hz]
Container_x_rmsd_rmsd_delta	50.155991521 [Hz]
Container_y_rmsd_rmsd_delta	50.155991521 [Hz]
Container_z_rmsd_rmsd_delta	50.155991521 [Hz]
Container_x_rmsd_rmsd_stddev	50.155991521 [Hz]
Container_y_rmsd_rmsd_stddev	50.155991521 [Hz]
Container_z_rmsd_rmsd_stddev	50.155991521 [Hz]
Container_x_rmsd_rmsd_rms	50.155991521 [Hz]
Container_y_rmsd_rmsd_rms	50.155991521 [Hz]
Container_z_rmsd_rmsd_rms	50.155991521 [Hz]
Container_x_rmsd_rmsd_mean	50.155991521 [Hz]
Container_y_rmsd_rmsd_mean	50.155991521 [Hz]
Container_z_rmsd_rmsd_mean	50.155991521 [Hz]
Container_x_rmsd_rmsd_std	50.155991521 [Hz]
Container_y_rmsd_rmsd_std	50.155991521 [Hz]
Container_z_rmsd_rmsd_std	50.155991521 [Hz]
Container_x_rmsd_rmsd_rmsd	50.155991521 [Hz]
Container_y_rmsd_rmsd_rmsd	50.155991521 [Hz]
Container_z_rmsd_rmsd_rmsd	50.155991521 [Hz]
Container_x_rmsd_rmsd_rmsd_max	50.155991521 [Hz]
Container_y_rmsd_rmsd_rmsd_max	50.155991521 [Hz]
Container_z_rmsd_rmsd_rmsd_max	50.155991521 [Hz]
Container_x_rmsd_rmsd_rmsd_min	50.155991521 [Hz]
Container_y_rmsd_rmsd_rmsd_min	50.155991521 [Hz]
Container_z_rmsd_rmsd_rmsd_min	50.155991521 [Hz]
Container_x_rmsd_rmsd_rmsd_center	50.155991521 [Hz]
Container_y_rmsd_rmsd_rmsd_center	50.155991521 [Hz]
Container_z_rmsd_rmsd_rmsd_center	50.155991521 [Hz]
Container_x_rmsd_rmsd_rmsd_delta	50.155991521 [Hz]
Container_y_rmsd_rmsd_rmsd_delta	50.155991521 [Hz]
Container_z_rmsd_rmsd_rmsd_delta	50.155991521 [Hz]
Container_x_rmsd_rmsd_rmsd_stddev	50.155991521 [Hz]
Container_y_rmsd_rmsd_rmsd_stddev	50.155991521 [Hz]
Container_z_rmsd_rmsd_rmsd_stddev	50.155991521 [Hz]
Container_x_rmsd_rmsd_rmsd_rms	

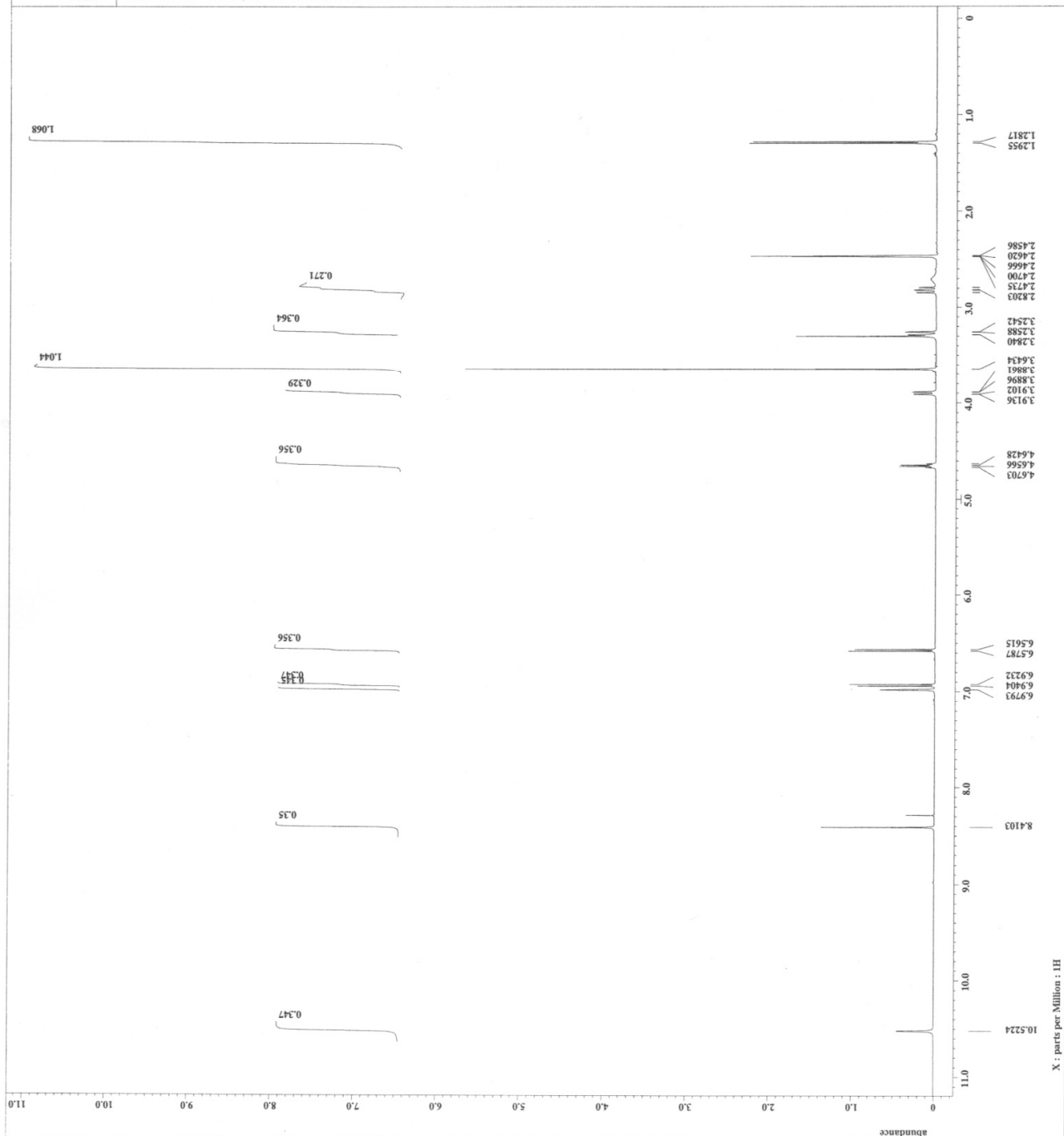
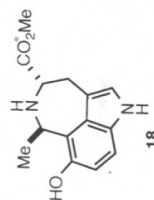


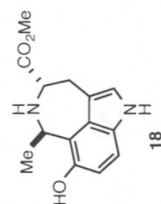
Derived from: Hyrtioerectine B Me-ester-

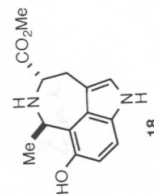
[illegible]

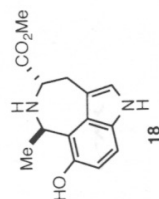
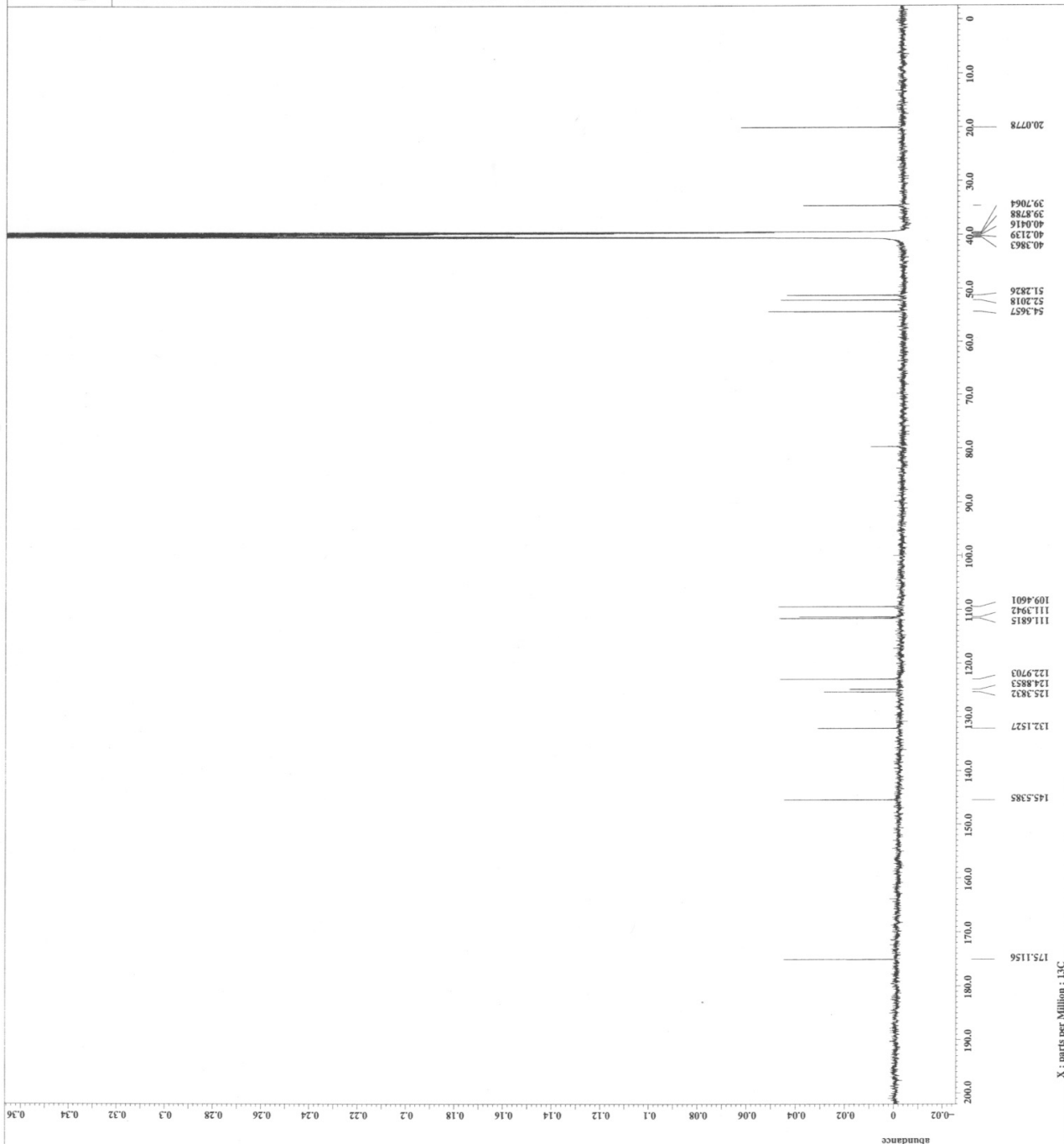
Derived from: Hyrtioerectine B Me-ester-

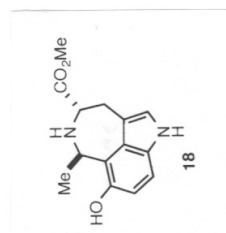


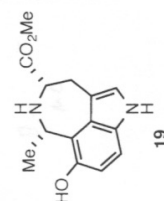




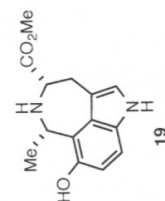


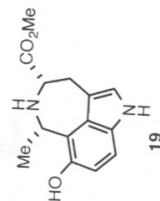






5 1



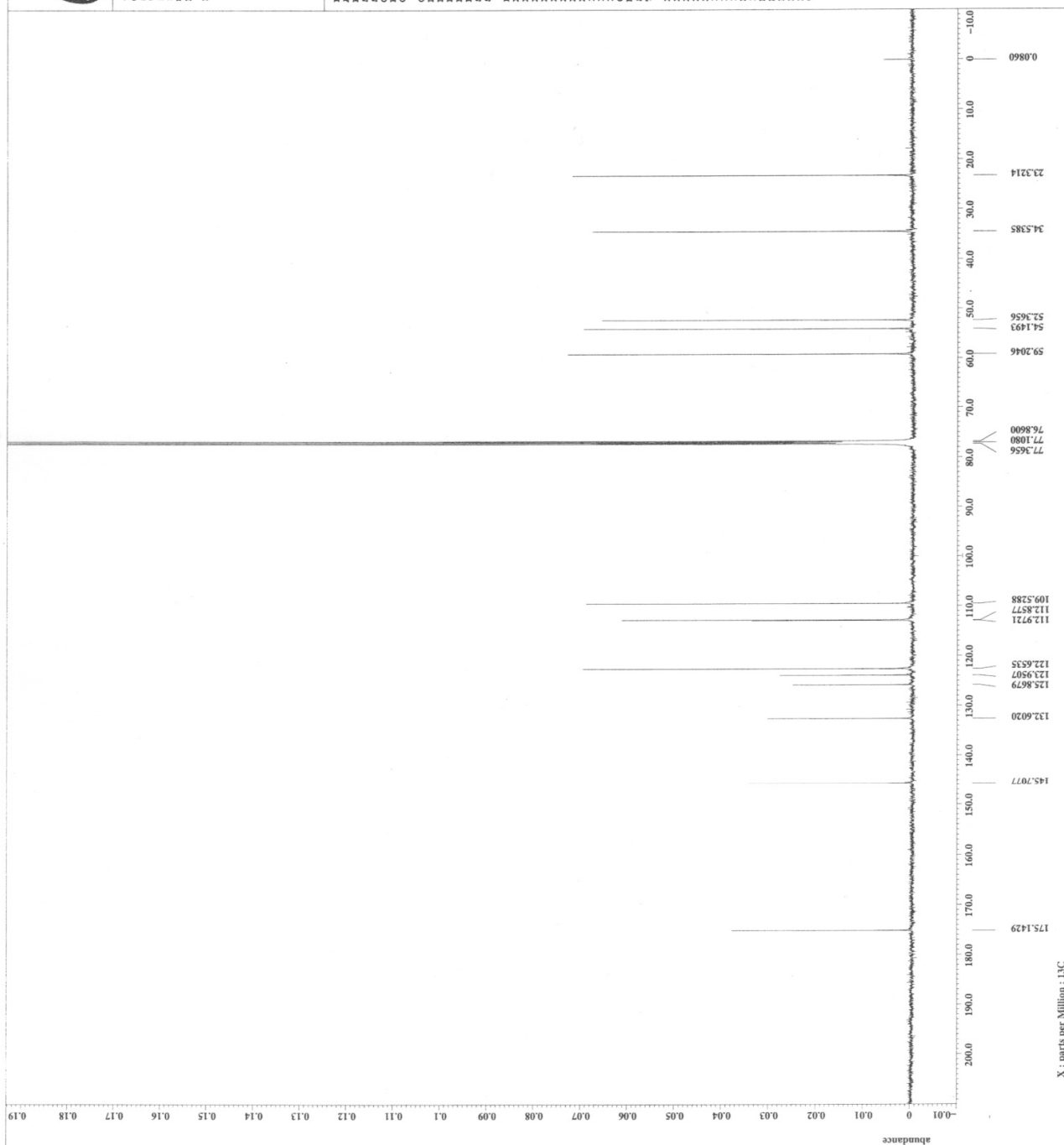
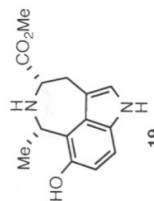


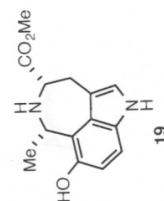
X : parts per Million : 1H

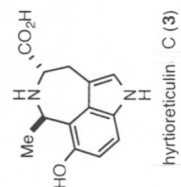


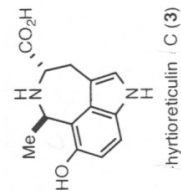
---- PROCESSING PARAMETERS ----
 de_maltese 0 : FALSE
 transoid3 0 : 80[°] : 100[°]
 zerofill 1 :
 machine : TRUE
 ppm
 Derived from: yema-16-12-06-3.jdf

=====
 File: yema-16-12-06-4.jdf
 Name: yema-16-12-06-4
 Experiment: single_pulse_dec
 Sample_id: S8621468
 Solvent: CHLOROFORM-D
 Date: 2016-08-20 21:20:21
 Revision: 1
 Current_time: 7-DEC-2016 08:24:44
 Comment: single pulse decouple
 Data_format: 1D COMPLEX
 File_size: 81.4
 Dim: 1
 Dim_units: [ppm]
 Dimensions: 1
 Spectrometer: DELTA 500
 Field_strength: 11.742379[G] (500[MH
 X_domain: 0.8336172[Hz]
 X_acq_duration: 13.3
 X_domain: 13C
 X_freq: 125.7652978[MHz]
 X_resolution: 32768
 X_points: 4
 X_prescans: 13858034[Hz]
 X_resolution: 39.3081761[MHz]
 X_sweep: 18
 X_domain: 18
 X_freq: 159.91521[MHz]
 X_resolution: 5.0[ppm]
 X_offset: FALSE
 Mod_return: 19092
 Total_scans: 19092
 X_resolution: 11.3[Hz]
 X_acq_time: 0.8336172[Hz]
 X_angle: 30[deg]
 X_atn: 3.9[deg]
 X_atn_dec: 21.238[db]
 X_atn_dec: 21.238[db]
 X_atn_dec: 21.238[db]
 X_atn_dec: TRUE
 Decoupling: 1[s]
 Initial_wait: 1[s]
 Noe_time: 2[Hz]
 Noe_gain: 54
 Relaxation_delay: 2[s]
 Relaxation_time: 23.3[sec]
 Temp_get:

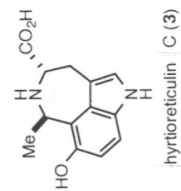


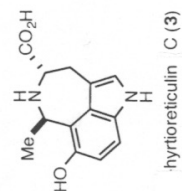






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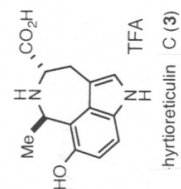






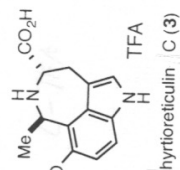
----- PROCESSING PARAMETERS -----
Date_UTC : 2016 04 22 15:53
freq_mhz : 500.1350989
solv : DMSO-d6
temp_cold3 : 0 [N] : 80 [N] : 100 [N]
temp_hot3 : 0 [N] : 100 [N]
zfc : 1 : TRUE : TRUE
machinephase
ppm
Derived from: hyrtioelectinC-TFA-1.jdf

Filename = hyrtioelectinC-TFA-4
AcqName = single_pulse-ex2
Sample_id = 8833089
Creation_time = 5-DEC-2016 04:22:53
Revision_time = 5-DEC-2016 09:31:39
Current_time = 5-DEC-2016 09:31:53
Comment = single_pulse
Data_format = 13-COMPLEX
Dir_title = 1M
Dir_units = [ppm]
Spectrum = ECA500
Spectrum = DELTA2_HMR
Field_strength = 11.7473575 [T] (500 MHz)
X_acq_duration = 1.74587904 [s]
X_domain = 20.15991521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_resolution = 0.5727737 [Hz]
X_sweep = 2.38438438 [kHz]
Xrr_domain = 500.15991521 [MHz]
Xrr_offset = 5.0 [ppm]
Xrr_domain = 20.15991521 [MHz]
Xrr_offset = 5.0 [ppm]
Clipped = FALSE
Scans = 8
Total_scans = 8
X_90_width = 11.8 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_pulse = 5.5 [us]
Xrr_mode = Off
Xrr_pulse = 1 [us]
Date_acq = 2016-12-05
Initial_wait = 1 [s]
Receiv_gain_delay = 54
Repetition_time = 6.74587904 [s]
Temp_get = 23.9 [dC]



Derived from: HyrtioerectineC-TFA-1.jdf

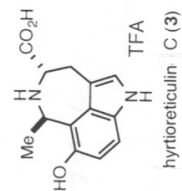
Filename	= PytloracineC-7FA
Author	= Data
Experiment	= Experiment
Sample	= SampleName.es2
Solvent	= DMSO-d6
Concentration	= 5-DMSO-2d6 04:22:53
Creation_time	= 5-DMSO-2d6 05:30:01
Current_time	= 5-DMSO-2d6 05:30:01
Comment	= sample_pulse
Data format	= 1D COMPLEX
Dir_name	= 13107
Dir_unit	= 13107
Dimensions	= 1 [ppm]
Site	= X
Spectrometer	= ECA500
Field_strength	= 121.7473579 [T] (500 [MHz]
Frequency	= 130.7597904 [Hz]
X_freq	= 500.159991521 [MHz]
X_resolution	= 16.84 [ppm]
X_points	= 16384
X_prescan	= 1
Y_resolution	= 0.57277773 [Hz]
Y_freq	= 130.7597904 [MHz]
Y_resolution	= 16.84 [ppm]
Y_points	= 16384
Y_prescan	= 1
Y_acquisition	= 500.159991521 [MHz]
Y_resolution	= 16.84 [ppm]
Y_points	= 16384
Y_prescan	= 1
Mod_return	= FALSE
Acq_start	= 0
Acq_end	= 0
Acq_secs	= 0
Acq_width	= 1.7 [us]
Acq_delay	= 1.7 [us]
Acq_pause	= 45 [sec]
Acq_sample	= 5 [us]
Acq_xatn	= 3.4 [dB]
Acq_yatn	= 3.4 [dB]
Acq_xoff	= 0 [us]
Acq_yoff	= 0 [us]
Acq_xmode	= Off
Acq_ymode	= Off
Acq_xphase	= 0 [deg]
Acq_yphase	= 0 [deg]
Acq_xpwr	= 54
Acq_ypwr	= 54
Acq_gain	= 54
Acq_delay	= 54 [us]
Acq_delay2	= 54 [us]
Acq_delay3	= 54 [us]
Acq_delay4	= 54 [us]
Acq_delay5	= 54 [us]
Acq_delay6	= 54 [us]
Acq_delay7	= 54 [us]
Acq_delay8	= 54 [us]
Acq_delay9	= 54 [us]
Acq_delay10	= 54 [us]
Acq_delay11	= 54 [us]
Acq_delay12	= 54 [us]
Acq_delay13	= 54 [us]
Acq_delay14	= 54 [us]
Acq_delay15	= 54 [us]
Acq_delay16	= 54 [us]
Acq_delay17	= 54 [us]
Acq_delay18	= 54 [us]
Acq_delay19	= 54 [us]
Acq_delay20	= 54 [us]
Acq_delay21	= 54 [us]
Acq_delay22	= 54 [us]
Acq_delay23	= 54 [us]
Acq_delay24	= 54 [us]
Acq_delay25	= 54 [us]
Acq_delay26	= 54 [us]
Acq_delay27	= 54 [us]
Acq_delay28	= 54 [us]
Acq_delay29	= 54 [us]
Acq_delay30	= 54 [us]
Acq_delay31	= 54 [us]
Acq_delay32	= 54 [us]
Acq_delay33	= 54 [us]
Acq_delay34	= 54 [us]
Acq_delay35	= 54 [us]
Acq_delay36	= 54 [us]
Acq_delay37	= 54 [us]
Acq_delay38	= 54 [us]
Acq_delay39	= 54 [us]
Acq_delay40	= 54 [us]
Acq_delay41	= 54 [us]
Acq_delay42	= 54 [us]
Acq_delay43	= 54 [us]
Acq_delay44	= 54 [us]
Acq_delay45	= 54 [us]
Acq_delay46	= 54 [us]
Acq_delay47	= 54 [us]
Acq_delay48	= 54 [us]
Acq_delay49	= 54 [us]
Acq_delay50	= 54 [us]
Acq_delay51	= 54 [us]
Acq_delay52	= 54 [us]
Acq_delay53	= 54 [us]
Acq_delay54	= 54 [us]
Acq_delay55	= 54 [us]
Acq_delay56	= 54 [us]
Acq_delay57	= 54 [us]
Acq_delay58	= 54 [us]
Acq_delay59	= 54 [us]
Acq_delay60	= 54 [us]
Acq_delay61	= 54 [us]
Acq_delay62	= 54 [us]
Acq_delay63	= 54 [us]
Acq_delay64	= 54 [us]
Acq_delay65	= 54 [us]
Acq_delay66	= 54 [us]
Acq_delay67	= 54 [us]
Acq_delay68	= 54 [us]
Acq_delay69	= 54 [us]
Acq_delay70	= 54 [us]
Acq_delay71	= 54 [us]
Acq_delay72	= 54 [us]
Acq_delay73	= 54 [us]
Acq_delay74	= 54 [us]
Acq_delay75	= 54 [us]
Acq_delay76	= 54 [us]
Acq_delay77	= 54 [us]
Acq_delay78	= 54 [us]
Acq_delay79	= 54 [us]
Acq_delay80	= 54 [us]
Acq_delay81	= 54 [us]
Acq_delay82	= 54 [us]
Acq_delay83	= 54 [us]
Acq_delay84	= 54 [us]
Acq_delay85	= 54 [us]
Acq_delay86	= 54 [us]
Acq_delay87	= 54 [us]
Acq_delay88	= 54 [us]
Acq_delay89	= 54 [us]
Acq_delay90	= 54 [us]
Acq_delay91	= 54 [us]
Acq_delay92	= 54 [us]
Acq_delay93	= 54 [us]
Acq_delay94	= 54 [us]
Acq_delay95	= 54 [us]
Acq_delay96	= 54 [us]
Acq_delay97	= 54 [us]
Acq_delay98	= 54 [us]
Acq_delay99	= 54 [us]
Acq_delay100	= 54 [us]
Acq_delay101	= 54 [us]
Acq_delay102	= 54 [us]
Acq_delay103	= 54 [us]
Acq_delay104	= 54 [us]
Acq_delay105	= 54 [us]
Acq_delay106	= 54 [us]
Acq_delay107	= 54 [us]
Acq_delay108	= 54 [us]
Acq_delay109	= 54 [us]
Acq_delay110	= 54 [us]
Acq	



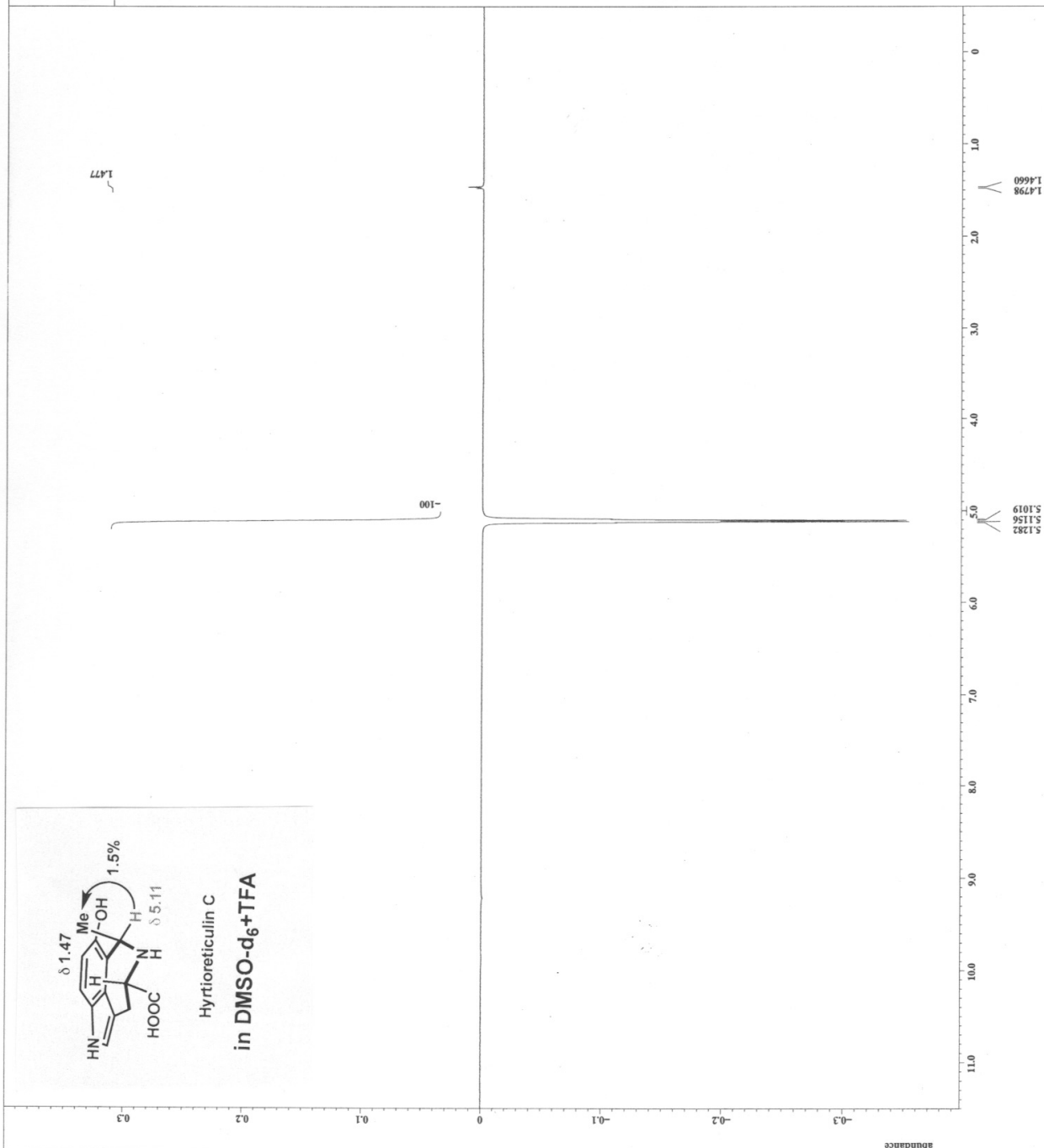


----- PROCESSING PARAMETERS -----
GC balance : 0 : FALSE
Sample mass : 0.0000 g
TropSolid : 0 [%] : 100 [%]
ZeroFill : 1
F2 C1 : TRUE
MachinePhase : TRUE
ppm
Derived from: HyrtioectineC-TFA-7.jdf

Filename = HyrtioectineC-TFA-8
Author =
Experiment =
SampleId = 485669
Solvent = DMSO-D6
Creation time = 6-DEC-2016 02:14:09
Creation date = 6-DEC-2016 02:14:09
Current time = 6-DEC-2016 07:22:28
Comment = single pulse decouple
Data format = ID COMPLEX
Data size = 26214
Dim size = 13C
Dim title =
Dimensions = X
Site = ECA500
Spectrometer = DELTA_NMR
Field strength = 11.747375 [T] (500 MHz)
X_acq_duration = 0.83361792 [s]
X_freq = 125.76529768 [MHz]
X_offset = 100 [ppm]
X_resolution = 4.27768
X_resolution = 1.19959034 [Hz]
X_resolution = 38.3081761 [MHz]
X_sweep = 500.15991521 [MHz]
Irr_freq = 5.0 [ppm]
Irr_offset = 1
ModReturn = 1
Scans = 19647
Total_scans = 19647
X_90_width = 11.3 [us]
X_acq_time = 0.83361792 [s]
X_delay = 5.5 [us]
X_echo = 5.5 [us]
X_pulse = 3.76666667 [us]
X_pulse_dec = 1.3 [us]
Irr_pulse = 21.238 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
P1 = 1
P2 = 1
Noe_time = 2 [s]
Acquisition = 2 [s]
Repetition_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get = 23.2 [dC]



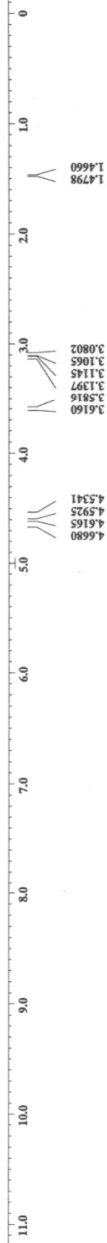
X : parts per Million : 13C



X : parts per Million : 1H

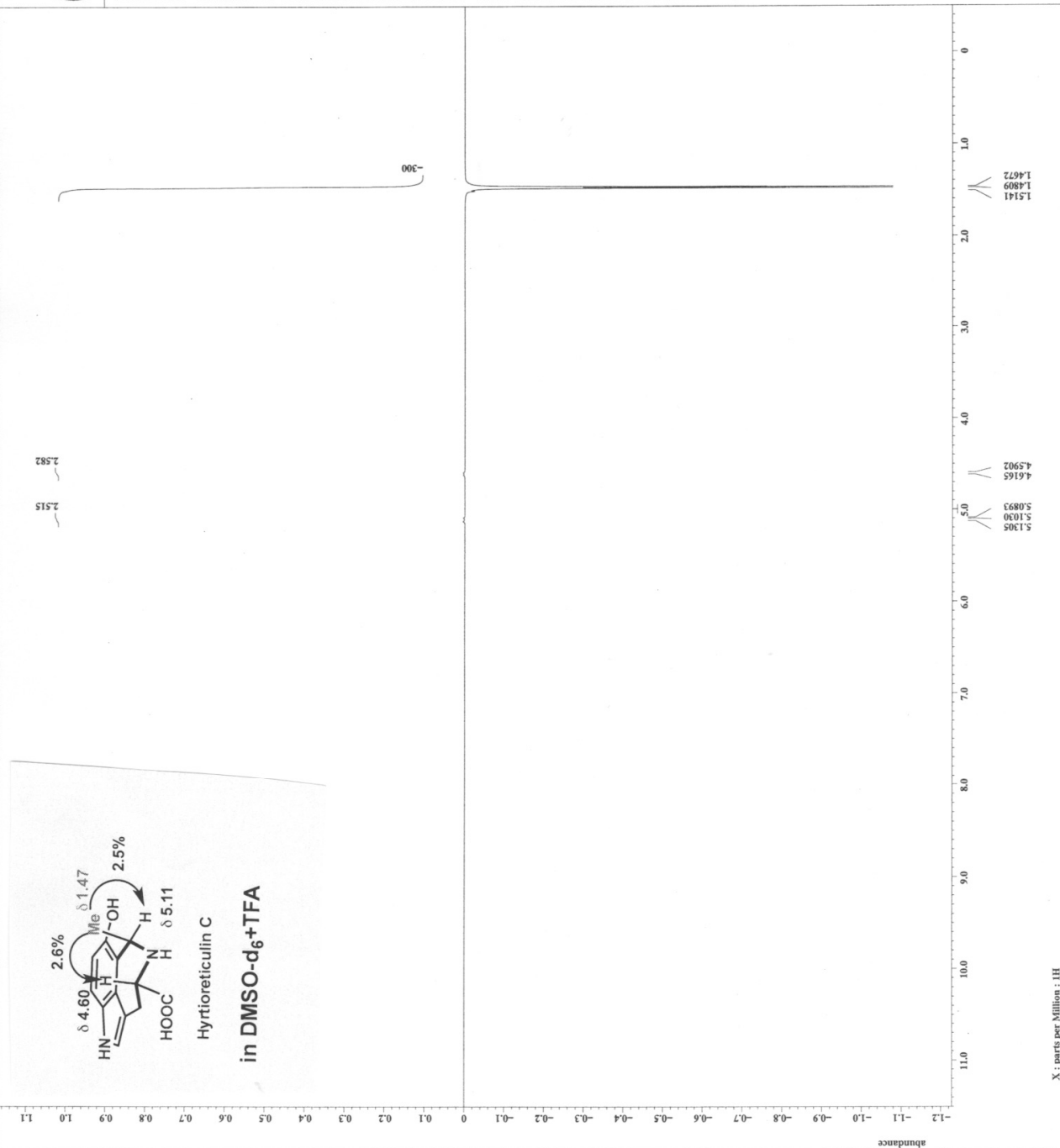


FileNames	= Birtlowinsulin_C17F1
Author	= daltla
Experiment	= Birtlowinsulin_C17F1
Solvent	= DMSO-d6
Creation_time	= 13-DEC-2015 20:41:50
Creation_time	= 13-DEC-2015 20:41:50
Current_time	= 20-DEC-2015 08:06:12
Current_time	= 20-DEC-2015 08:06:12
Constant	= DPMSE NOE 1d
Content	= 1D COMPLEX
D1a_delay	= 13107
D1a_delay	= 13107
D1a_units	= [µs]
Dimensions	= X 30 640
Spectrometer	= MZT422_NMR
Field_strength	= 1.42936421 [T] (500.1M)
Frequency	= 18.74429121 [MHz]
Freq_offset	= 495.13191398 [MHz]
Freq_offset	= 495.13191398 [MHz]
F2_points	= 10184
F2_points	= 10184
F2_resolution	= 2.4664949 [Hz]
F2_resolution	= 2.4664949 [Hz]
F2_sweep	= 9.28677563 [kHz]
F2_sweep	= 9.28677563 [kHz]
F2_domain	= 18.13191398 [MHz]
F2_domain	= 18.13191398 [MHz]
F2_offset	= 5 [µmol]
F2_offset	= 5 [µmol]
F2_freq	= 495.13191398 [MHz]
F2_freq	= 495.13191398 [MHz]
F2_phase	= FALSE
F2_phase	= FALSE
F2_Clipped	= 1
F2_Clipped	= 1
Mod_return	= 1
Mod_return	= 1
Total_scans	= 1024
Total_scans	= 1024
Acq_time	= 1.76433912 [s]
Acq_time	= 1.76433912 [s]
Acq_n	= 3.6160
Acq_n	= 3.6160
Acq_pulse	= 13.7 [µs]
Acq_pulse	= 13.7 [µs]
Obs_sel_180	= 20 [µs]
Obs_sel_180	= 20 [µs]
Obs_sel_atn	= 51.736 [dB]
Obs_sel_atn	= 51.736 [dB]
Obs_sel_offset	= 0.000000 [ppm]
Obs_sel_offset	= 0.000000 [ppm]
Obs_sel_alp	= 5.1156 [ppm]
Obs_sel_alp	= 5.1156 [ppm]
Tr_mode	= OF2
Tr_mode	= OF2
Grd_1_offset	= 1 [ms]
Grd_1_offset	= 1 [ms]
Grd_1_amp	= 20 [µs]
Grd_1_amp	= 20 [µs]
Grd_2_amp	= 30 [µs]
Grd_2_amp	= 30 [µs]
Grd_3_amp	= 1 [ms]
Grd_3_amp	= 1 [ms]
Grd_4_offset	= 0.1 [ms]
Grd_4_offset	= 0.1 [ms]
Grd_4_phase	= 23.98 [°]
Grd_4_phase	= 23.98 [°]
Initial_wait	= 50
Initial_wait	= 50
Recvr_gain	= 1 [s]
Recvr_gain	= 1 [s]
Relaxation_delay	= 7 [s]
Relaxation_delay	= 7 [s]
Relaxation_time	= 1.76433912 [s]
Relaxation_time	= 1.76433912 [s]
Retention	= 20.42 [min]
Retention	= 20.42 [min]

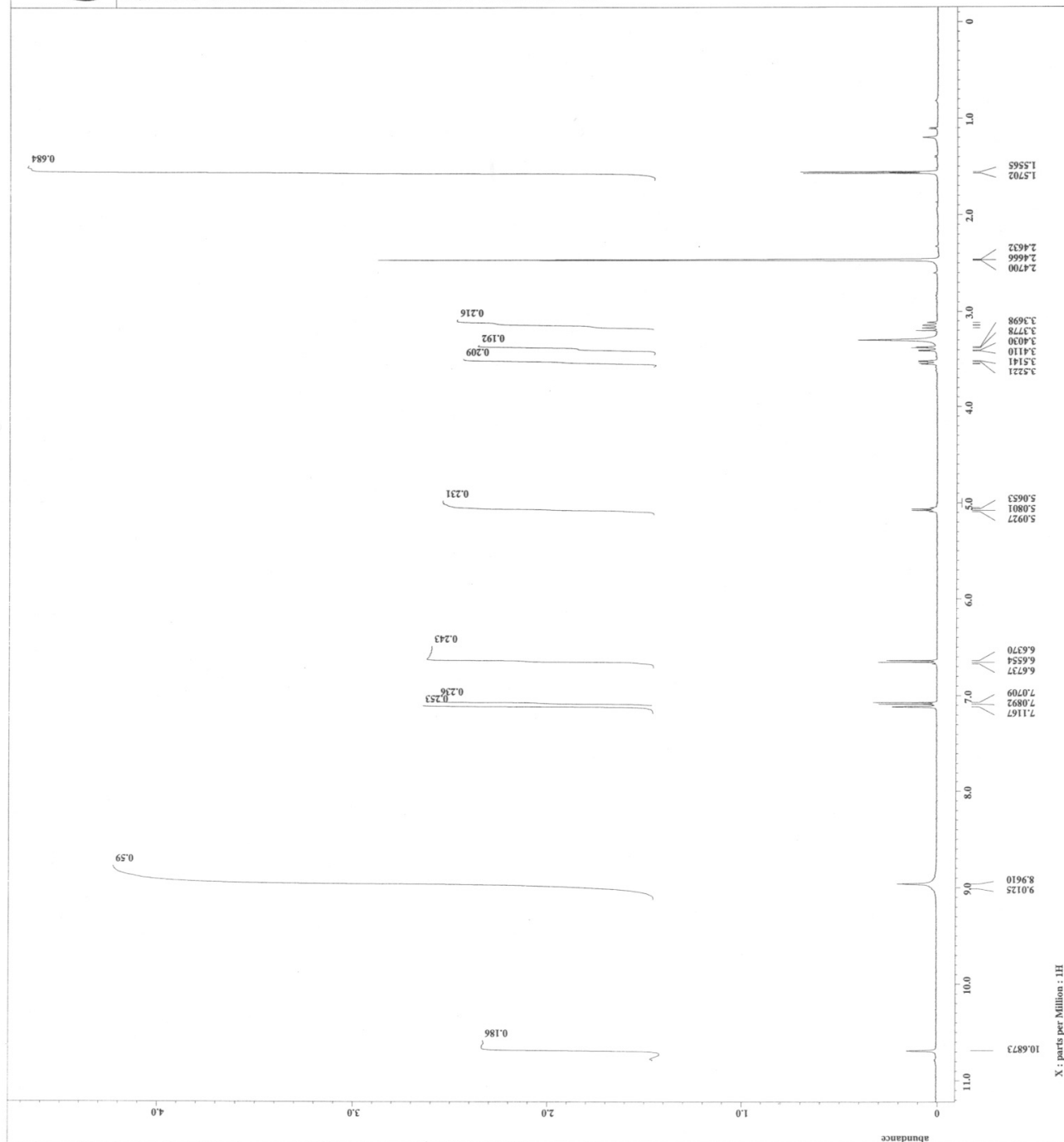
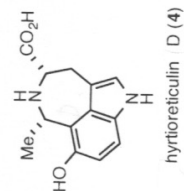


X : parts per Million : 1H

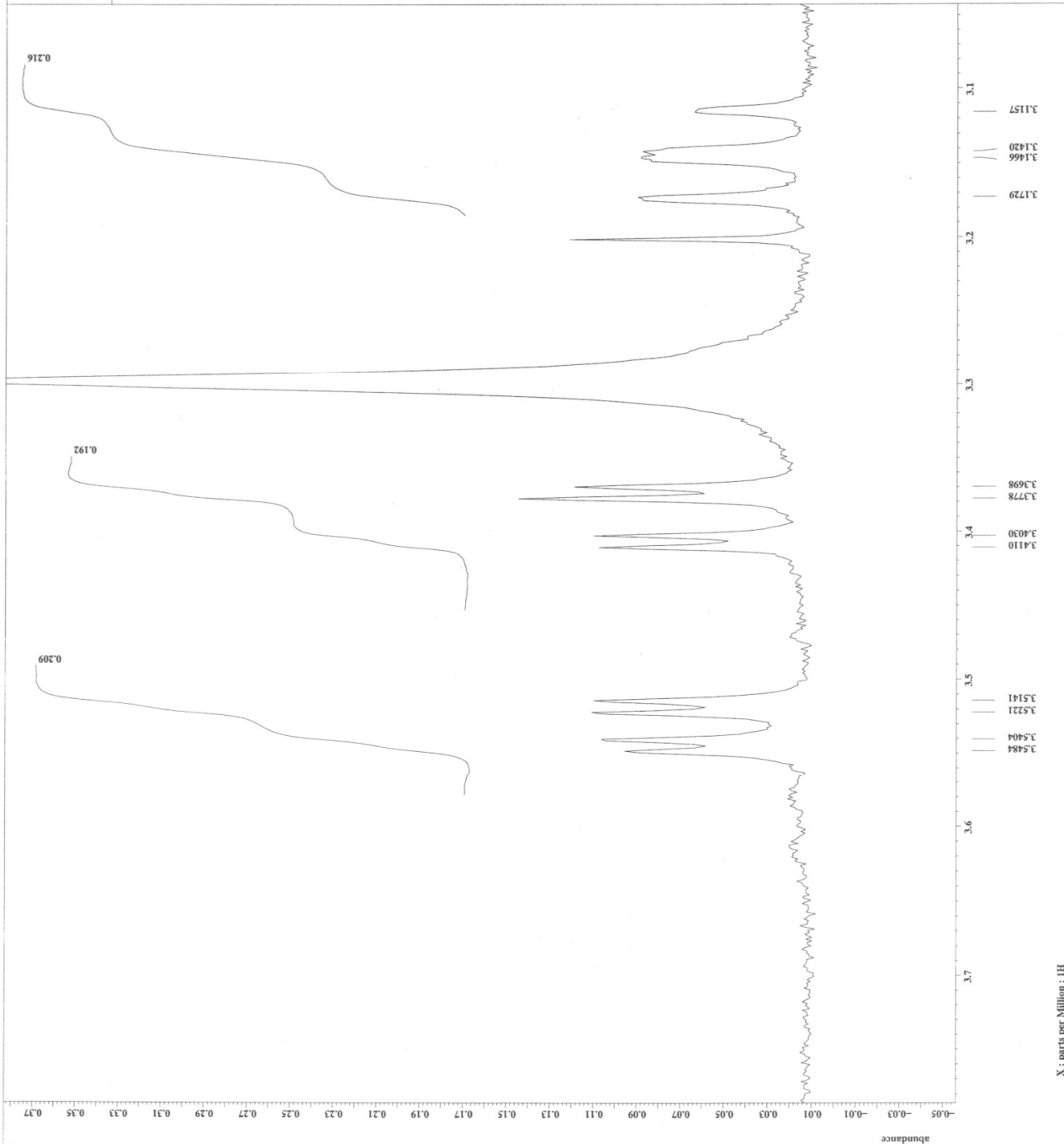
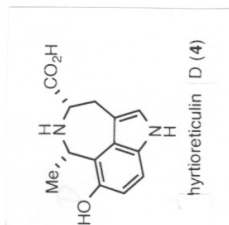
[illegible]



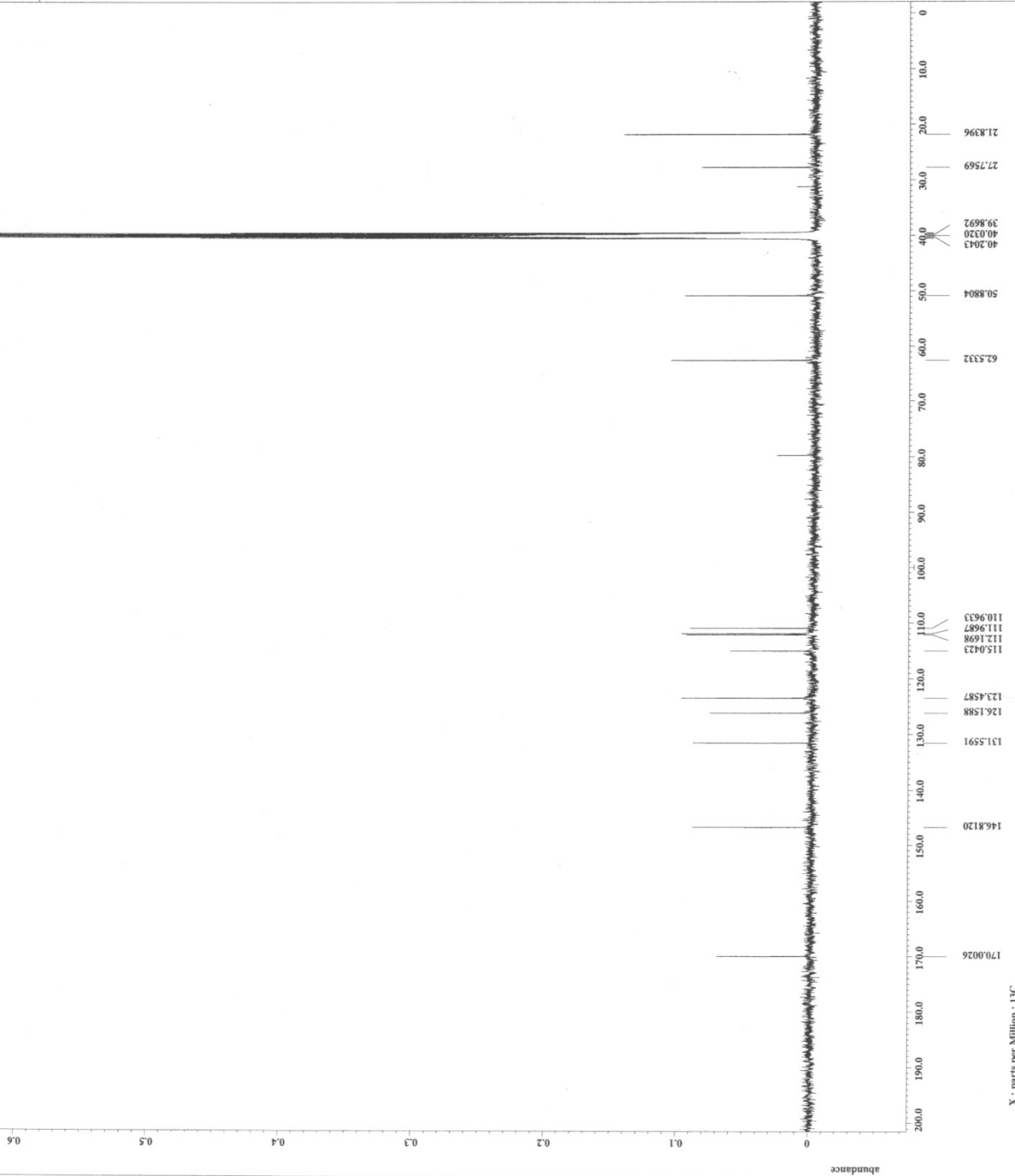
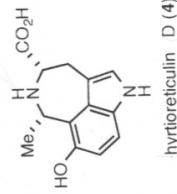
File name = Hyrtioreticulic C.TFA
 Experiment =
 Sample_id = nos_1d_dpfgse.ex
 Date_acq = 20-DEC-2016 02:00:17
 Creation_time = 20-DEC-2016 08:07:36
 Revision_time = 20-DEC-2016 08:07:55
 Current_time =
 Content = DFGSE NOE 1d
 Data_format = ID COMPLEX
 Data_title = 1D
 Dia_units = [ppm]
 Dimensions = FCA 500
 Size = DELTA2_MNR
 Spectrometer =
 Field_strength = 11.42026421(T) (500[M]
 X_acq_duration = 1.76422912[s]
 X_domain = 1H -13131398[NHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.5668198[Hz]
 X_sweep = 9.28677563[NHz]
 Xrr_domain = 1H -13131398[NHz]
 Xrr_offset = 5[ppm]
 Tri_domain = 1H -13131398[NHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1034
 Total_scans = 1024
 X_acq_time = 1.76422912[s]
 X_pulse = 12.7[us]
 Xrr_mode_180 = Off[ms]
 Obs_sel_atn = 53.756[db]
 Obs_sel_offset = 1.4798[ppm]
 Obs_sel_offset = 1.4798[ppm]
 Obs_sel_offset = 1.4798[ppm]
 Tri_mode = Off
 Data_presat = 1[ms]
 Grad_1_amp = 20[%]
 Grad_2_amp = 1[ms]
 Grad_3_amp = 1[ms]
 Grad_4_amp = 10[%]
 Grad_5_amp = 1[ms]
 Grad_6_amp = 1[ms]
 Grad_shape = SINE
 Initial_wait = 1[s]
 Mix_time = 0.5[s]
 Relaxation_delay = 7[s]
 Repetition_time = 8.76422912[s]
 Temp_gvt = 21.9[OC]



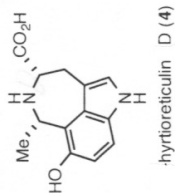
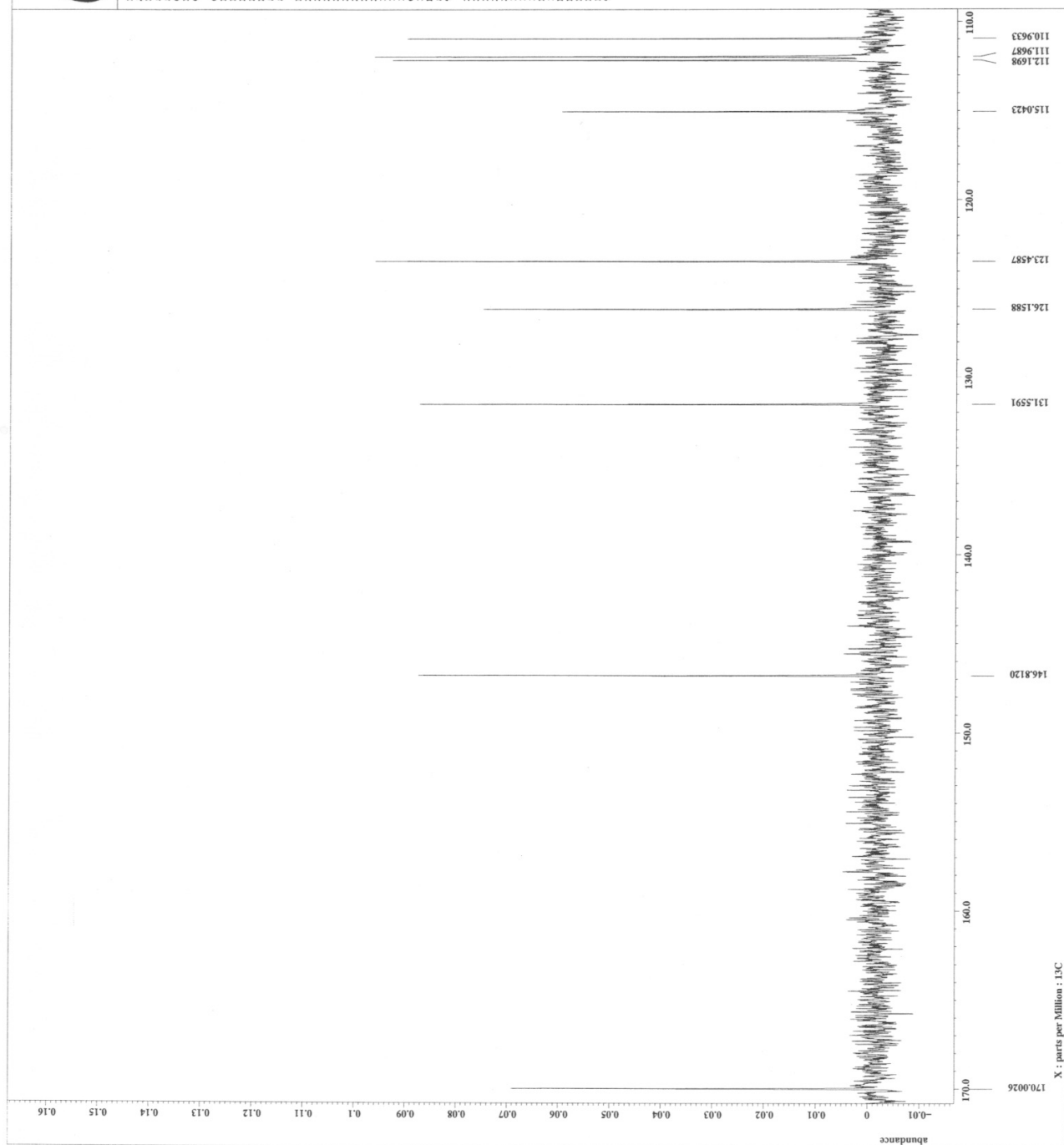
Filename = Hyrtioreticulin-D-1ra
 Sample = single_pulse_en2
 Sample_id = 8836339
 Experiment = 6-DEC-2016 09:55:52
 Revision_time = 6-DEC-2016 10:10:10
 Current_time = 6-DEC-2016 10:10:12
 Content = single_pulse
 Data_format = 1D COMPLEX
 Data_size = 13107
 Dia_units = [ppm]
 Dimensions = 512
 Size = ECA 500
 Spectrometer = DELTA2 NMR
 Field_strength = 11.62926421[T] (500[M]
 X_acq_duration = 1.76422912[s]
 X_domain = 1H
 X_offset = 165.13191398[MHz]
 X_points = 512
 X_resolution = 16384
 X_sweep = 0.5668198[Hz]
 Irr_domain = 1H
 Irr_offset = 165.13191398[MHz]
 Tri_domain = 1H
 Tri_offset = 165.13191398[MHz]
 Tri_resolution = 512
 Tri_offset = 165.13191398[MHz]
 Clipped = FALSE
 Recv_return = 8
 Total_scans = 8
 X_90_width = 12.7[us]
 X_acq_time = 1.76422912[s]
 X_angle = 45[deg]
 X_delay = 6.35[us]
 X_pulse = OFF
 Irr_mode = OFF
 Irr_delay = 1[us]
 Data_preset = FALSE
 Initial_wait = 1[s]
 Recv_gain = 48
 Repetition_delay = 6.76422912[s]
 Repetition_time = 20.6[dc]
 Temp_get =

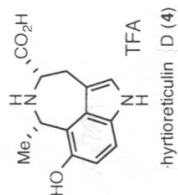
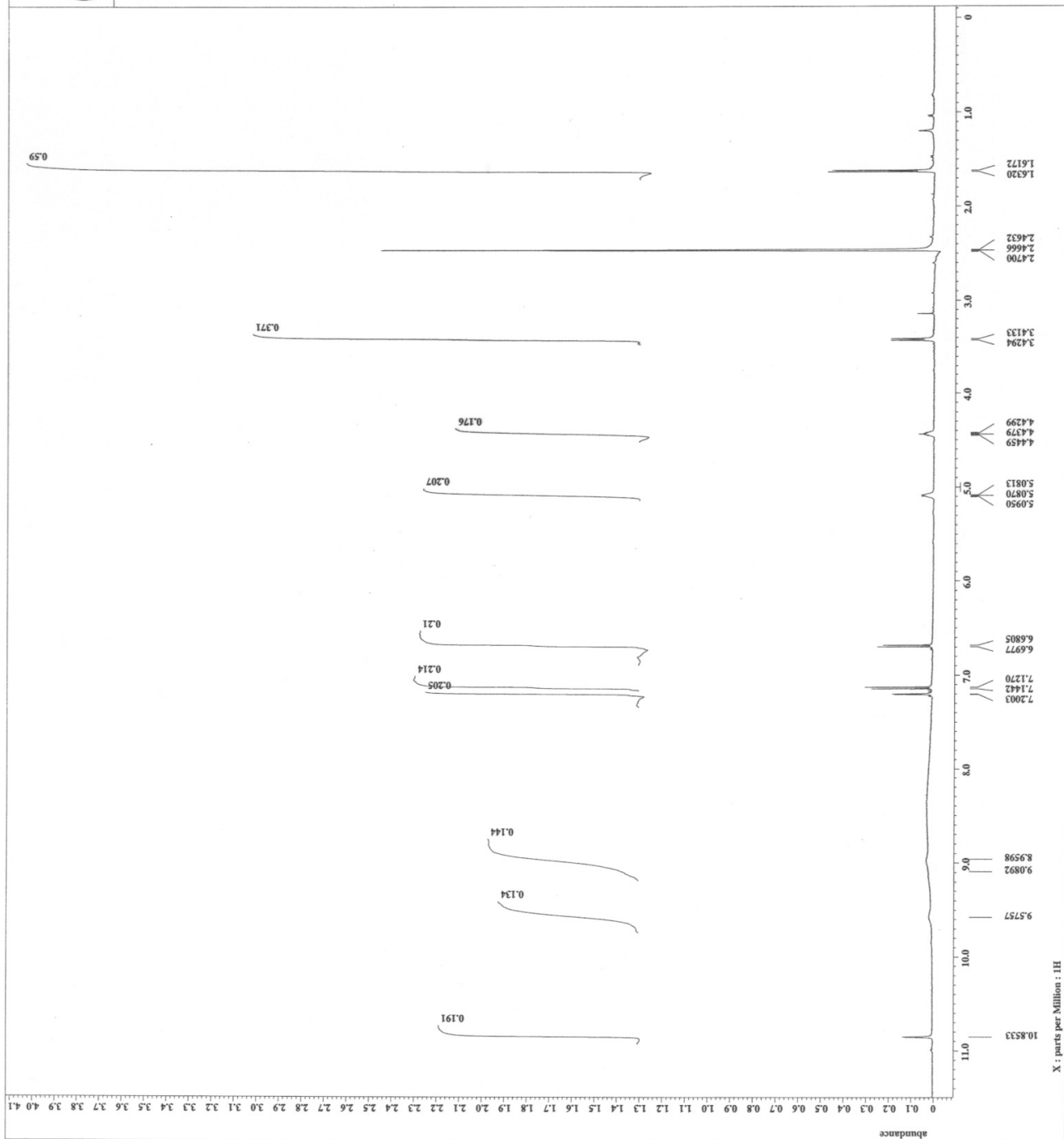


Filename = hyrtioreticulind2_cop
 Author = Delta
 Experiment = single_pulse_dec
 Date_acq = 2016-12-08
 Solvent = DMSO-d6
 Creation_time = 8-DEC-2016 14:24:22
 Revision_time = 8-DEC-2016 14:36:17
 Current_time = 8-DEC-2016 14:39:10
 Content = single pulse decouple
 Data format = 1D F2
 Data size = 26214
 Dim title = 13C
 Dim units = [ppm]
 Dimensions = 1
 Site = ECA 500
 Spectrometer = DELTA2_MMR
 Field_strength = 11.62926421(T) (500 MHz)
 X_acq_duration = 0.838860(s)
 X_domain = 13C
 X_offset = 5010059 [MHz]
 X_points = 100 [ppm]
 X_resolution = 32768
 X_sweep = 1.1920929 [Hz]
 X_sweep_rate = 39.0625 [kHz]
 Irr_domain = 485.1131398 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Modulated_wave_copy = TRUE
 Mod_return = 1
 Scans = 2489
 Total_scans = 2489
 X_90_width = 10.6 [us]
 X_acq_time = 0.838860(s)
 X_resolution = 32768
 X_resolution_ppm = 9.8 [dB]
 X_pulse = 3.5333333 [us]
 Irr_atn_dec = 20 [dB]
 Irr_atn_swept = 20 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Nutation_wait = 1 [s]
 Noe_time = 2 [s]
 Repetition_delay = 5 [s]
 Repetition_time = 2.838860(s)
 Temp_get = 21.6 (°C)

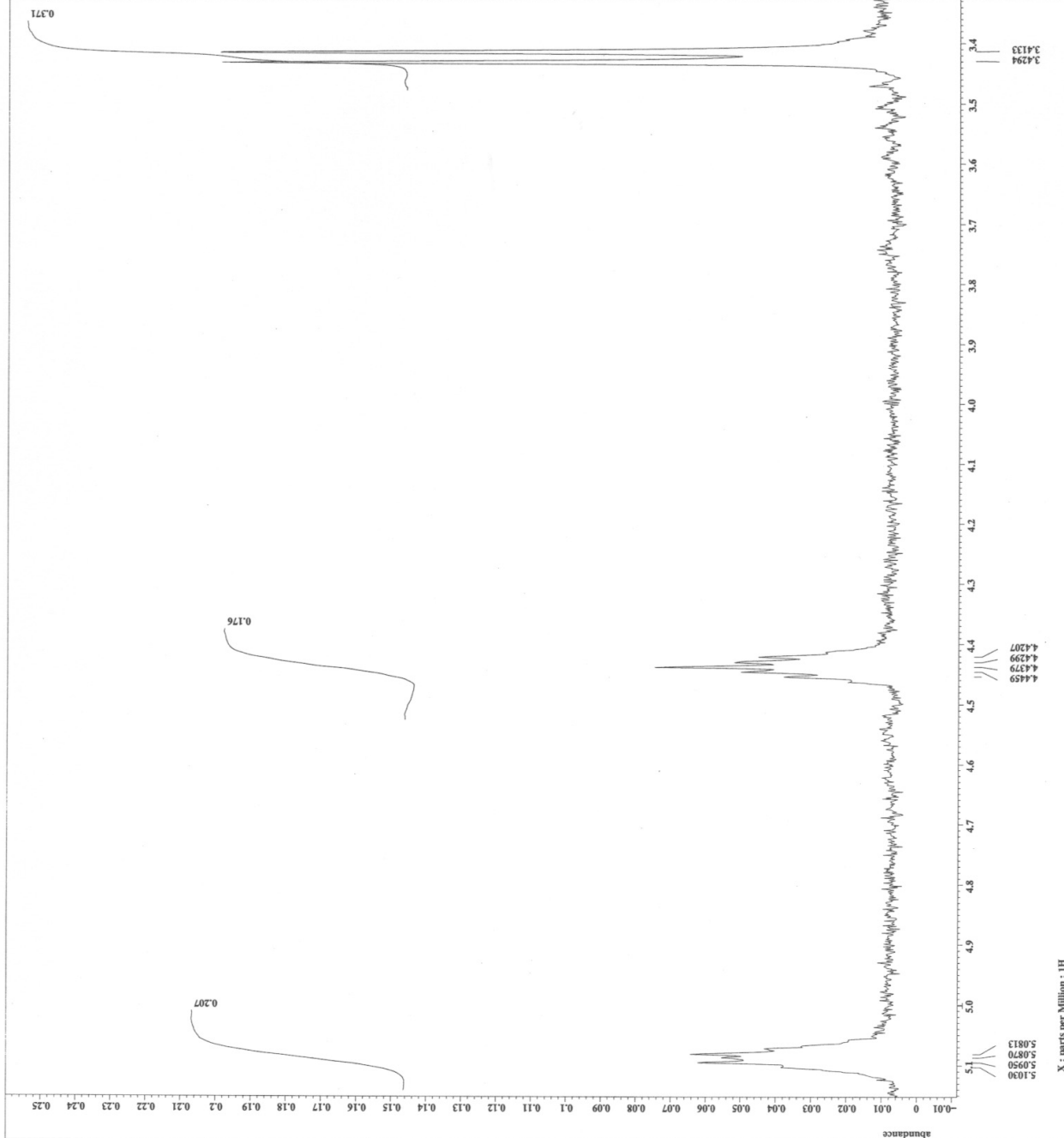
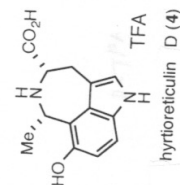


X : parts per Million : 13C

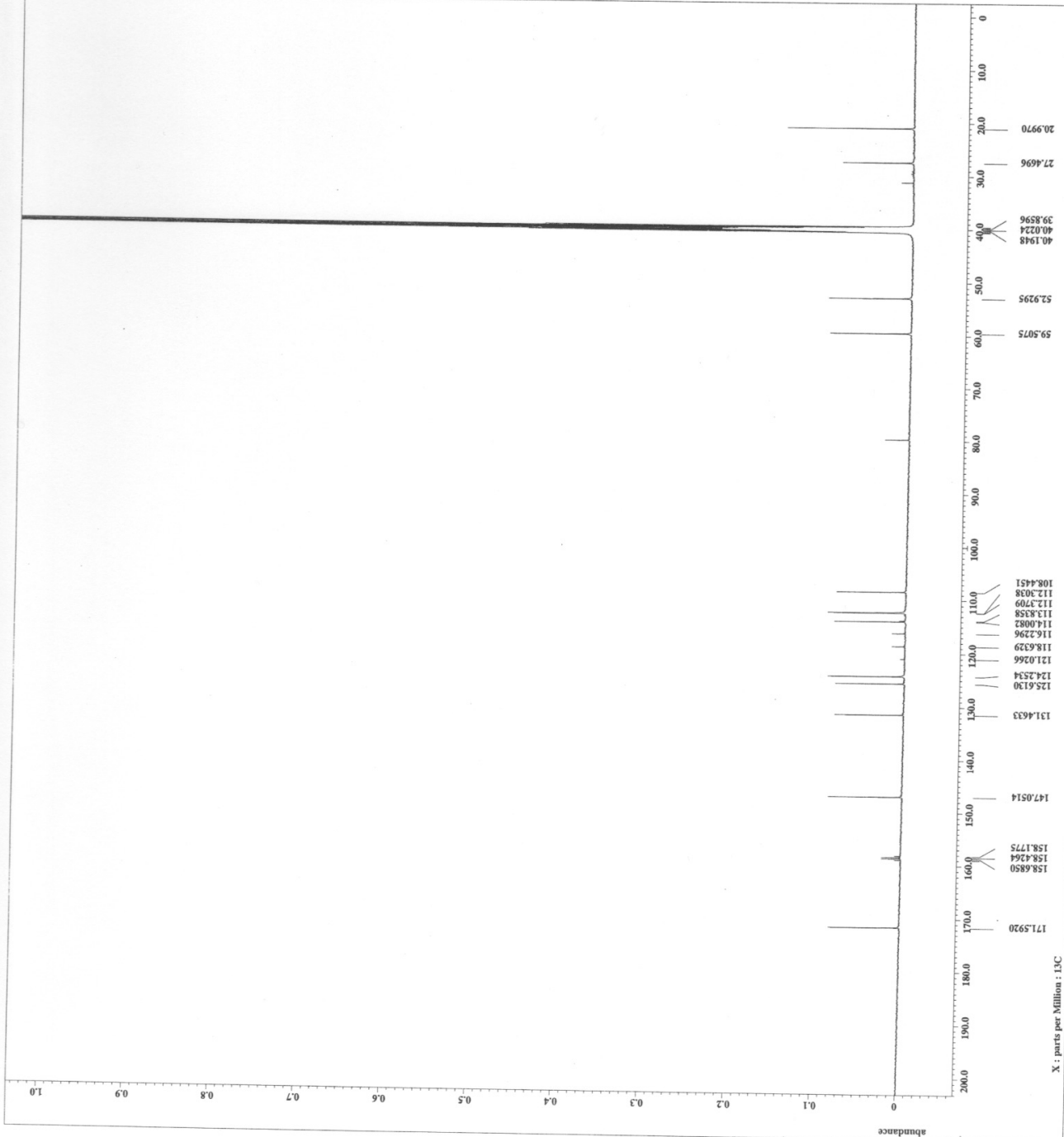
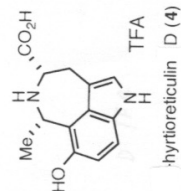




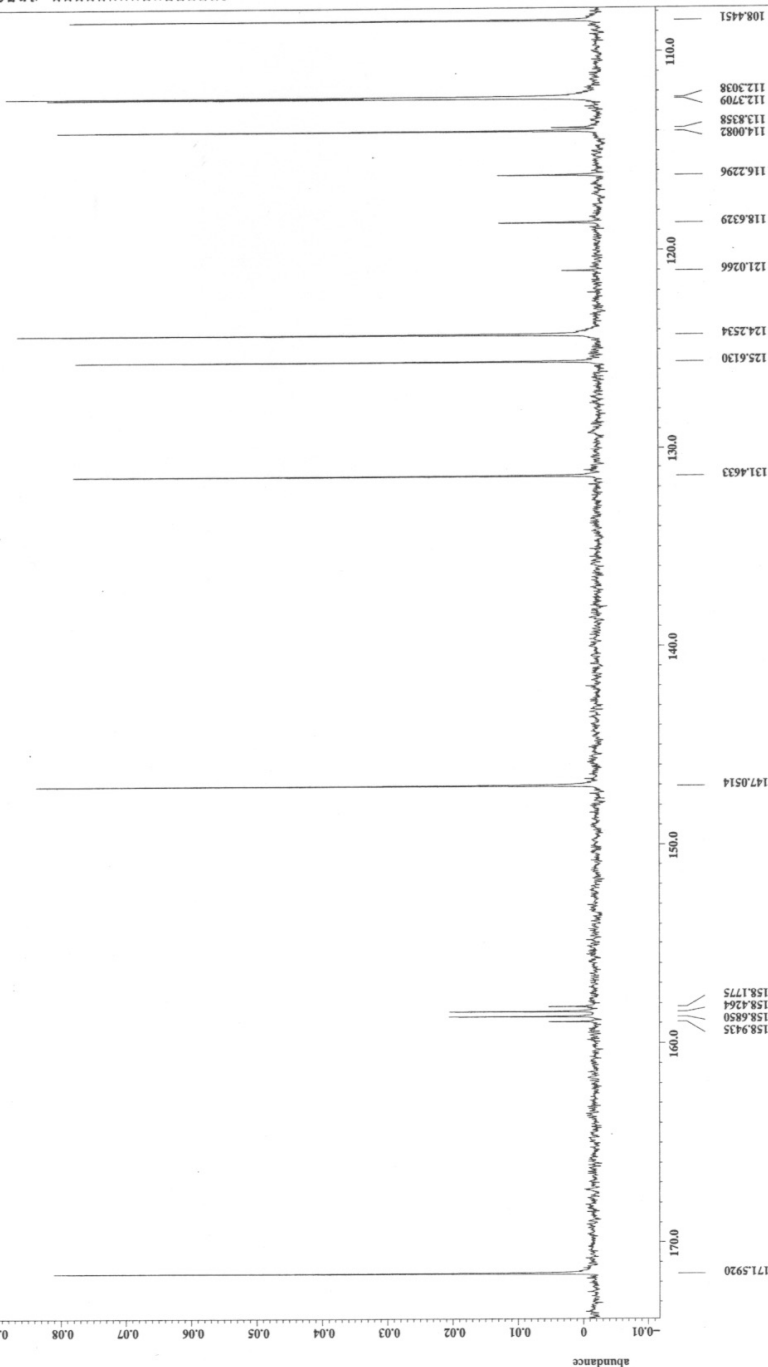
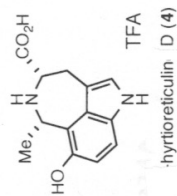
Filename = hyrtioreticulin-D2-TF
 Author = delta
 Experiment = single_pulse.ac2
 Solvent = DMSO-d6
 Creation_time = 10-MCC-2016 14:23:10
 Acquisition_time = 10-MCC-2016 14:23:12
 Current_time = 10-MCC-2016 14:23:22
 Content = 1D COMPLEX
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_unit = [mm]
 Dimensions = X
 Site = RCA 500
 Spectrometer = spectrometer
 Field_strength = 11.62936421 [T] [500 MHz]
 X_resolution = 11.62936421 [Hz]
 X_domain = 1H [644229121s]
 X_freq = 495.13191398 [MHz]
 X_offset = 13394
 X_pulses = 13394
 X_prescans = 1
 X_resolution = 1.866194 [Hz]
 X_resolution = 9.28677563 [Hz]
 Irr_domain = 1H
 Irr_freq = 595.13191398 [MHz]
 Tri_domain = 1H
 Tri_freq = 495.13191398 [MHz]
 Mod_return = 1
 Total_scans = 8
 X_90_width = 12.7 [us]
 X_acq_time = 1.764229121s
 X_angle = 45 [deg]
 X_offset = 13394
 X_pulse = 6.35 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dam_presat = PRSG
 Initial_wait = 1[s]
 Recv_gain_delay = 5[s]
 Repetition_time = 6.764229121s
 Temp_get = 21.4 [deg]



File name	Wf10rte06collin-025-27
Author	Galila
Experiment	Superimposed
Software	EMSD-06
Solvent	DMSO-d6
Creation time	12-DEC-2016 08:10:18
Creation date	2016-12-12
Current time	12-DEC-2016 08:10:27
Current date	2016-12-12
Content	100% pulse decouple
Data format	1D CompZxtk
Dir name	20214
Dir path	20214
D1C units	13C
Dimensions	X
Site	13C
Spectrometer	ECA 500
Field_strength	500.13 MHz
Field_frequency	125.7606421 [T] 500 [M]
X_freq	125.7606421 [MHz]
X_channel	13C
Y_freq	125.7606421 [MHz]
Y_channel	13C
Z_freq	125.7606421 [MHz]
Z_channel	13C
X_points	2727 [pts]
Y_points	4
Z_points	4
Acquisition	1.1920929 [Hz]
Relaxation	1H 0.622 [Hz]
Excitation	495.13191396 [MHz]
Excitation_freq	495.13191396 [MHz]
Excitation_channel	1H
Decoupled	FALSE
Mod_return	1
Mod_name	0001
Procr_name	22881
K0_offset	0.0 [Hz]
K0_width	30.0 [Hz]
K0_sqc_time	30 [sec]
K_angle	9.4 [deg]
K_offset	9.4 [deg]
K_width	323 [us]
Arrr_atn_dec	20.8 [dB]
Arrr_atn_spc	20.8 [dB]
Arrr_atn_rec	20.8 [dB]
Decoupling	WALTZ
Initial_waltz	1 [s]
Recr_gain	2101
Recr_time	60 [s]
Relaxation_delay	1 [s]
Relaxation_time	31 [sec]
Temp_set	21.7 [deg]



Filename	Content
Author	Content
Experiment	Content
Sample_id	Content
Solvent	Content
Creation	Content
Revision	Content
Current_t	Content
Dim1	Content
Dim2	Content
Dim3	Content
Dim4	Content
Dim5	Content
Dim6	Content
Dim7	Content
Dim8	Content
Dim9	Content
Dim10	Content
Dim11	Content
Dim12	Content
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Dim163	Content
Dim164	Content
Dim165	Content
Dim166	Content
Dim167	Content
Dim168	Content



X : parts per Million : 13C

in DMSO-d₆+TFA

1.95

The logo for JOEAL features the word "JOEAL" in a bold, sans-serif font. To the left of the text is a stylized graphic element consisting of a triangle with a circle inside it, and a line that loops around the triangle and ends in a small circle, resembling a stylized 'J' or a mechanical part.

```

-----
PROCESSING PARAMETERS
mc_balance: 0 : FALSE
exp: 0.2 [Hz] : 0.0 [s]
arazozeoid: 0 [s] : 80 [s] : 100 [%]
zerofill: 1
fft: 1 : TRUE : TRUE
ppm
Phase: 167 : 0 : 50 [%]

```

Derived from: Hyrtioreticulin D+TFA-4.jd

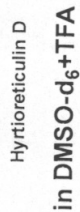
[illegible]

001-

1.6354
1.6205

6580'S
9660'S

X : parts per Million : 1H

The logo for JOEAL, featuring the word "JOEAL" in a bold, sans-serif font, with a stylized graphic element resembling a triangle or a stylized letter 'A' integrated into the letter 'A'.

```

----- PROCESSING PARAMETERS -----
dc balance: 0 : false
sorp : 0.3 [Hz] : 0.0 [s]
trapzoid: 0 [%] : 80 [%] : 100 [%]
zerofill : 1
fft : 1 : TRUE : TRUE
pwm
phase : 164 : 0 : 50 [%]

```

Derived from: Myrtiozoculin D-TFA

Filename	F:\vireticolin.D\F7F
Author	= data
Experiment	= nom_id_0fsgse.exe
SampleId	= NOM-D6
Solvent	= 15-DEC-2016 20:49:48
Creation_time	= 20-DEC-2016 08:51:53
Current_time	= 20-DEC-2016 08:53:02
Comment	
Data_format	= SPX025_NMR id
Dia_name	= 11_CPM2D_X
Dia_title	= 1107
Dimensions	= [ppm]
Size	= EGAS600
Appoperator	= DZS2A1_NMR
Field_strength	= 11.7473579 [G] (500 [MHz])
Acquisition	= 11.747357904 [s]
X_domain	= 50.15999452 [MHz]
Y_freq	= 13.8 [Hz]
X_offset	= 13.8 [Hz]
X_center	= 2
X_resolution	= 0.37277737 [Hz]
X_resolution_min	= 18.358488 [Hz]
X_freq	= 50.15999452 [MHz]
Y1_domain	= 18.358 [ppm]
Y1_freq	= 50.15999452 [MHz]
Y1_offset	= 18.358 [ppm]
Y1_resolution	= 0.37277737 [Hz]
Y1_resolution_min	= 18.358 [ppm]
Y1_center	= 2
Mod_return	= 124
Total_points	= 124
X_acq_time	= 1.747357904 [s]
X_pulse	= 11.8 [us]
Xir_psd	= OFZ
Xir_psd_0	= 54.235 [dB]
Obs_ref_sfn	= 1.6354 [ppm]
Obs_ref_offset	= 1.6354 [ppm]
Obs_ref_gain	= 1.6354 [ppm]
Obs_ref_slp	= OFZ
Xir_psd_max	= 54.235 [dB]
Grad_1_amp	= 66 [mT/m]
Grad_2_amp	= 90 [mT/m]
Grad_3_amp	= 1 [mT/m]
Grad_4_amp	= 30 [mT/m]
Grad_shape	= SINE
Initial_wait	= 1[s]
Nucv_gain	= 50 [s]
Relaxation_delay	= 7[s] ppgg904[s]
Relaxation_time	= 22.1 [s]

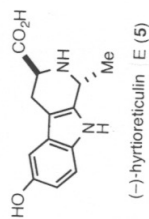


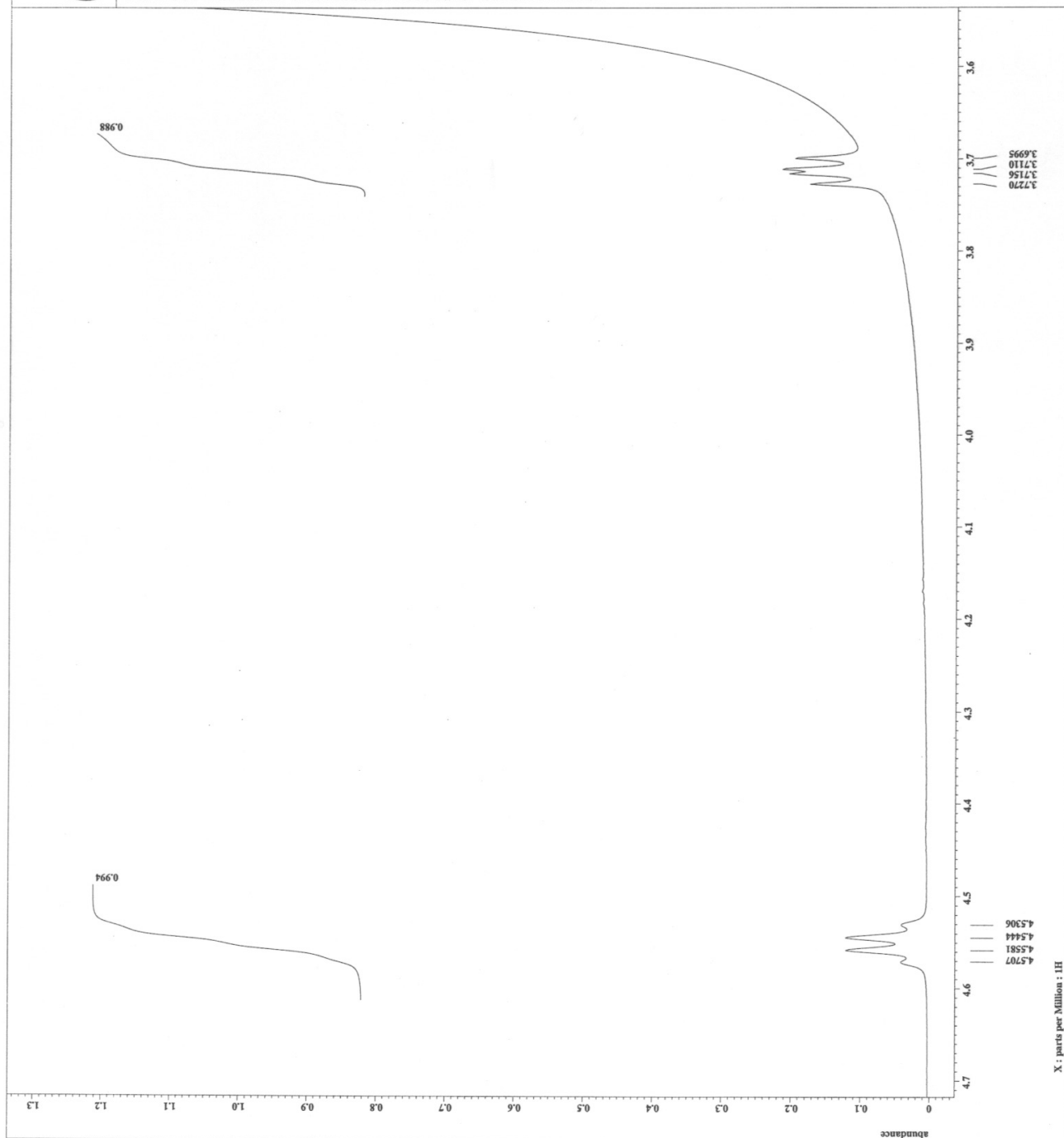
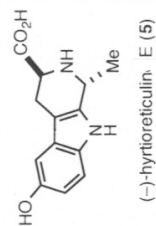
X : parts per Million : 1H




```
----- PROCESSING PARAMETERS -----
ddc_balance : 0 : FALSE
ddc_exp : 0.2 [Hz] : 0.0 [s]
trazodol : 0.0 [g] : 0.0 [g]
trazodol3 : 0.0 [g] : 80 [g] : 100 [g]
serofill : 1
fft : 1 : TRUE : TRUE
ppm
phase : -193 : 0 : 50 [°]
Derived from: Hyrtioreticulin D-TFA-6.jd
```

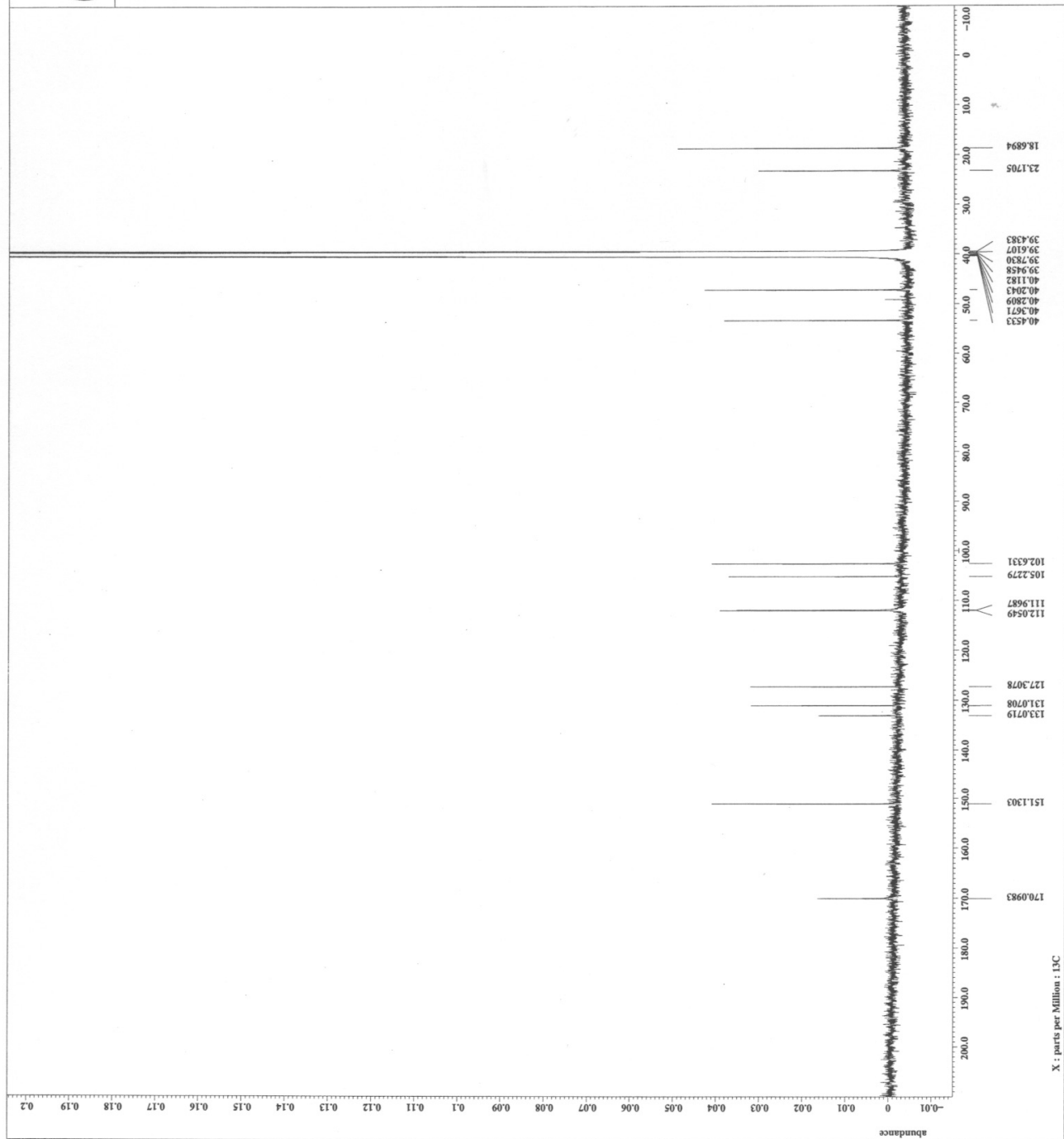
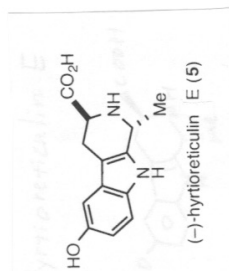
[illegible]

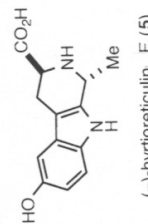








(-)-hyrtioretulin E (5)

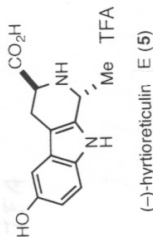


[illegible]

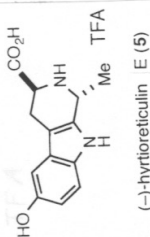


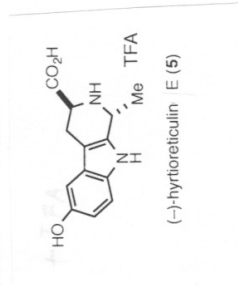

(-)-hyrtioreticulin E (5)

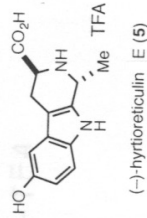
(-)-hyrtioreticulinal E (5)

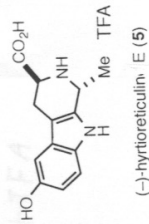
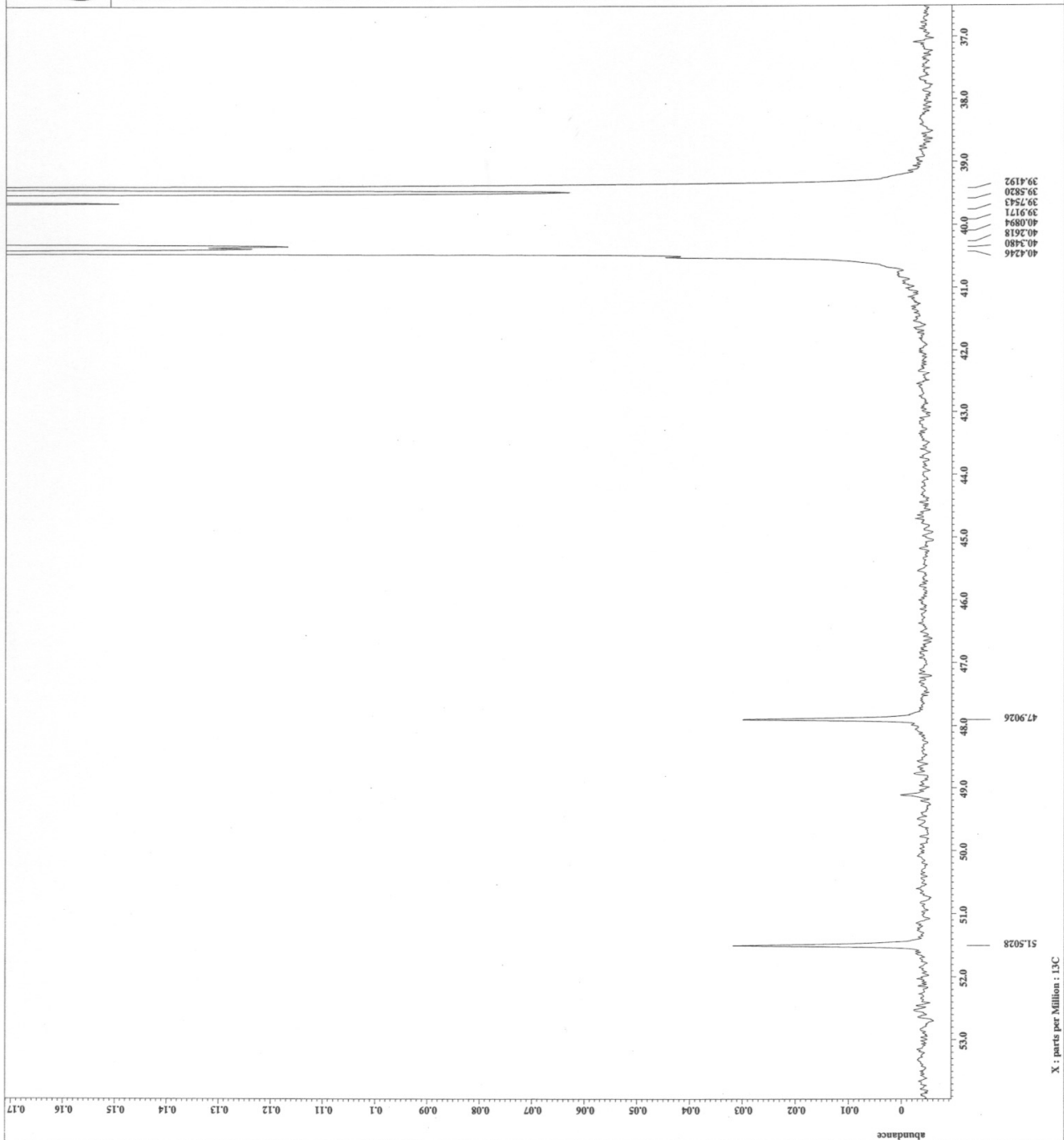


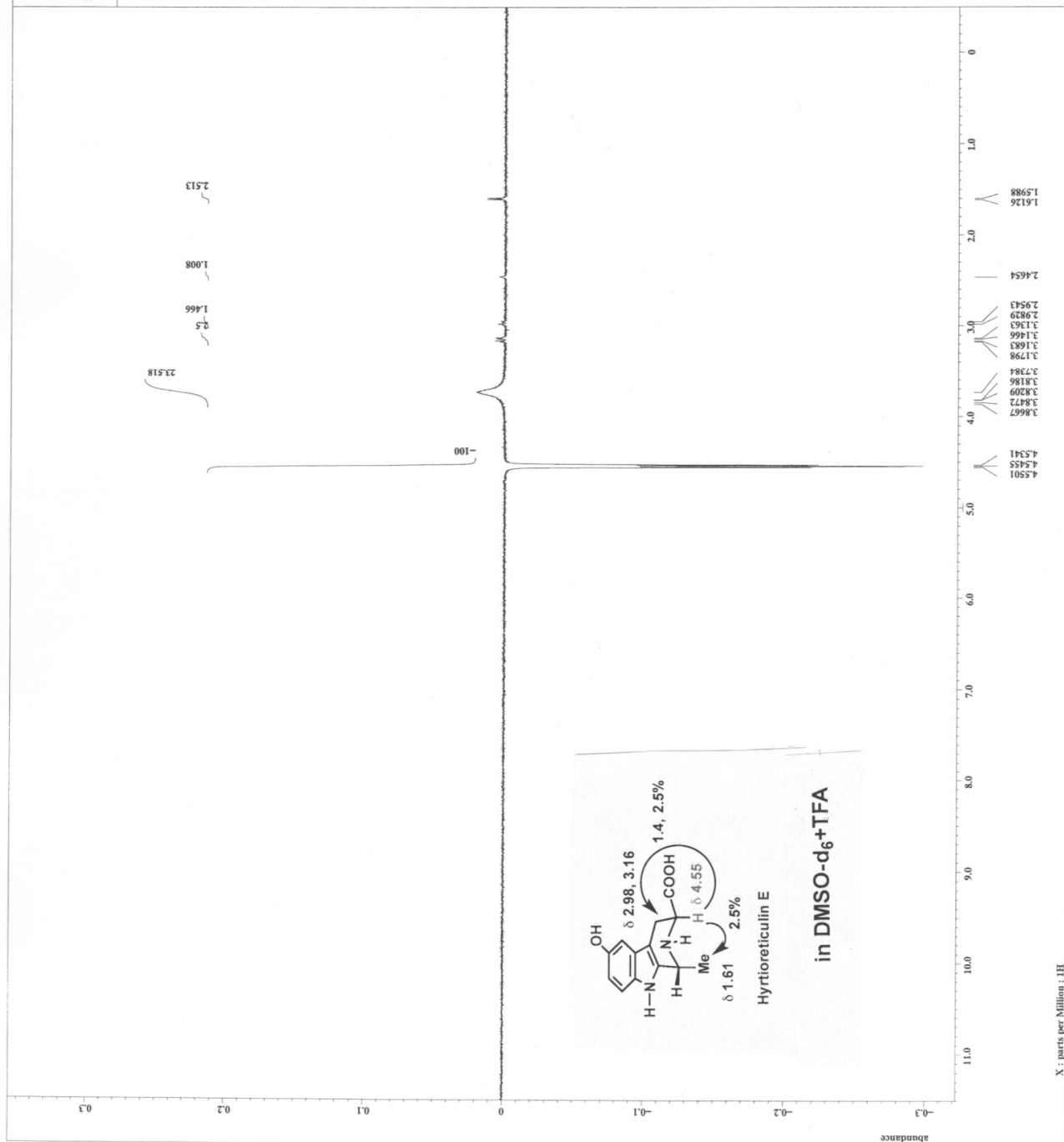
X : parts per Million : 1H





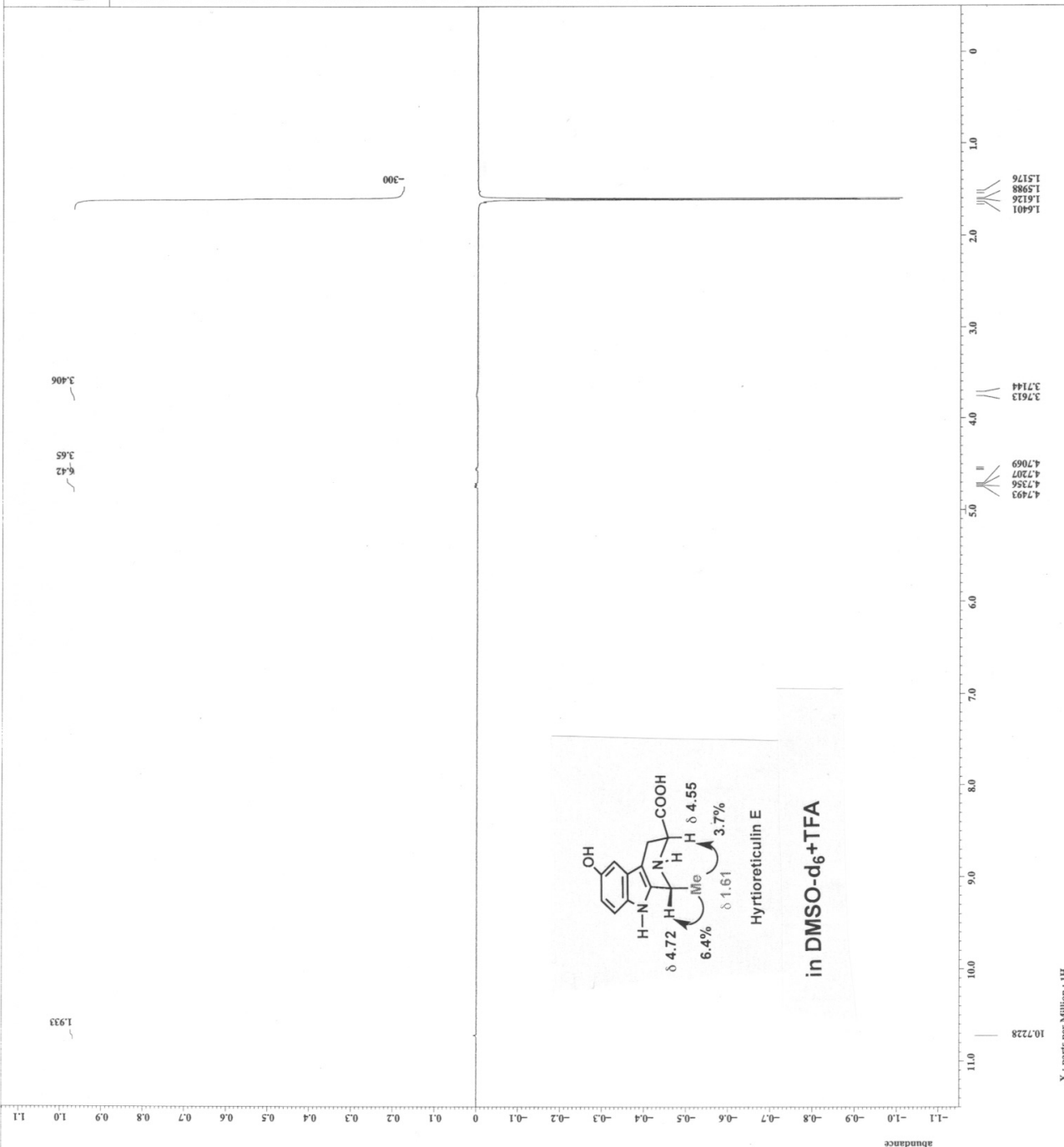


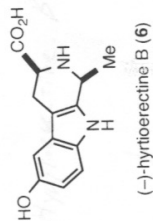


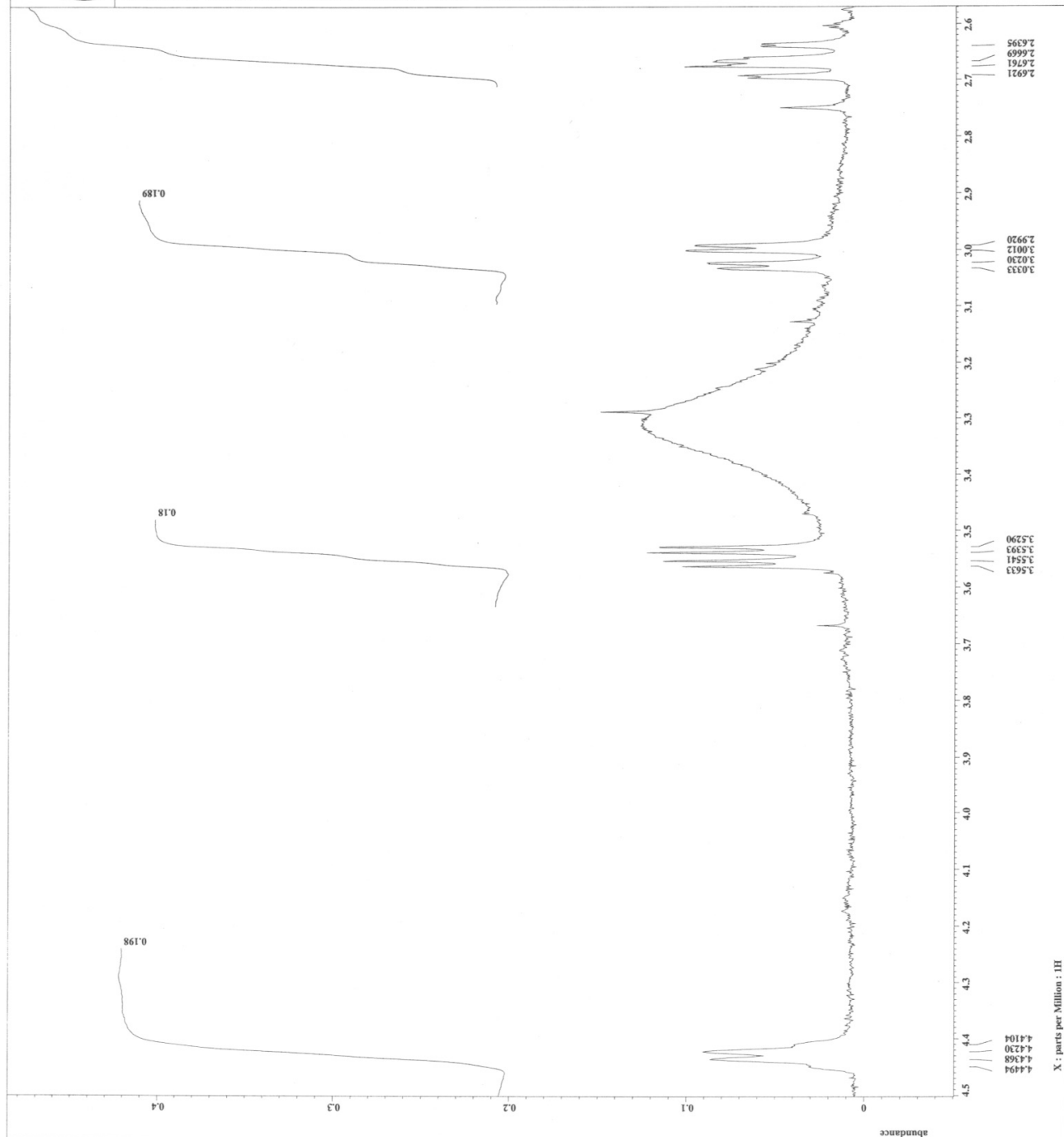
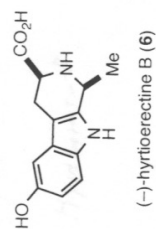




Filename = Hyrtioreticulin E.TFA
Sample_id = 1
Experiment = noa_1d_0pfgse_en
Sample_id = YANA
Date_acq = 2016-11-14 11:43:52
Creation_time = 21-DEC-2016 18:01:28
Revision_time = 21-DEC-2016 18:01:35
Current_time =
Content = DPPQSE NOE 1d
Data_format = ID COMPLEX
Data_size = 11.43 MB
Dm_title =
Dm_units = [ppm]
Dimensions = 500
Spectrometer = DELTA2_MMR
Field_strength = 11.43296431[G] (500[M]
X_acq_duration = 1.76422512[s]
X_domain = 1H
X_freq = 495.1313398[MHz]
X_points = 16384
X_resolution = 2.866198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.1313398[MHz]
Irr_mode = 1
Irr_pulse = 12.7[us]
Irr_shape = 1
Irr_time = 23.795[us]
Obs_sel_offset = 1.6126[ppm]
Obs_sel_shape = GAUSS
Obs_sel_sweep = 10[ppm]
Tri_mode = off
Dante_preset = FALSE
Grad_1_amp = 10[%]
Grad_1_shape = 1[ms]
Grad_2_amp = 30[%]
Grad_2_shape = 10[%]
Grad_3_amp = 0.1[ms]
Grad_3_shape = 1[ms]
Grad_recovery = 1[ms]
Mix_time = 0.5[s]
Recovery_gain = 50
Recovery_delay = 6.76422512[s]
Repetition_time = 59.6[s]
Temp_set = 50[degC]

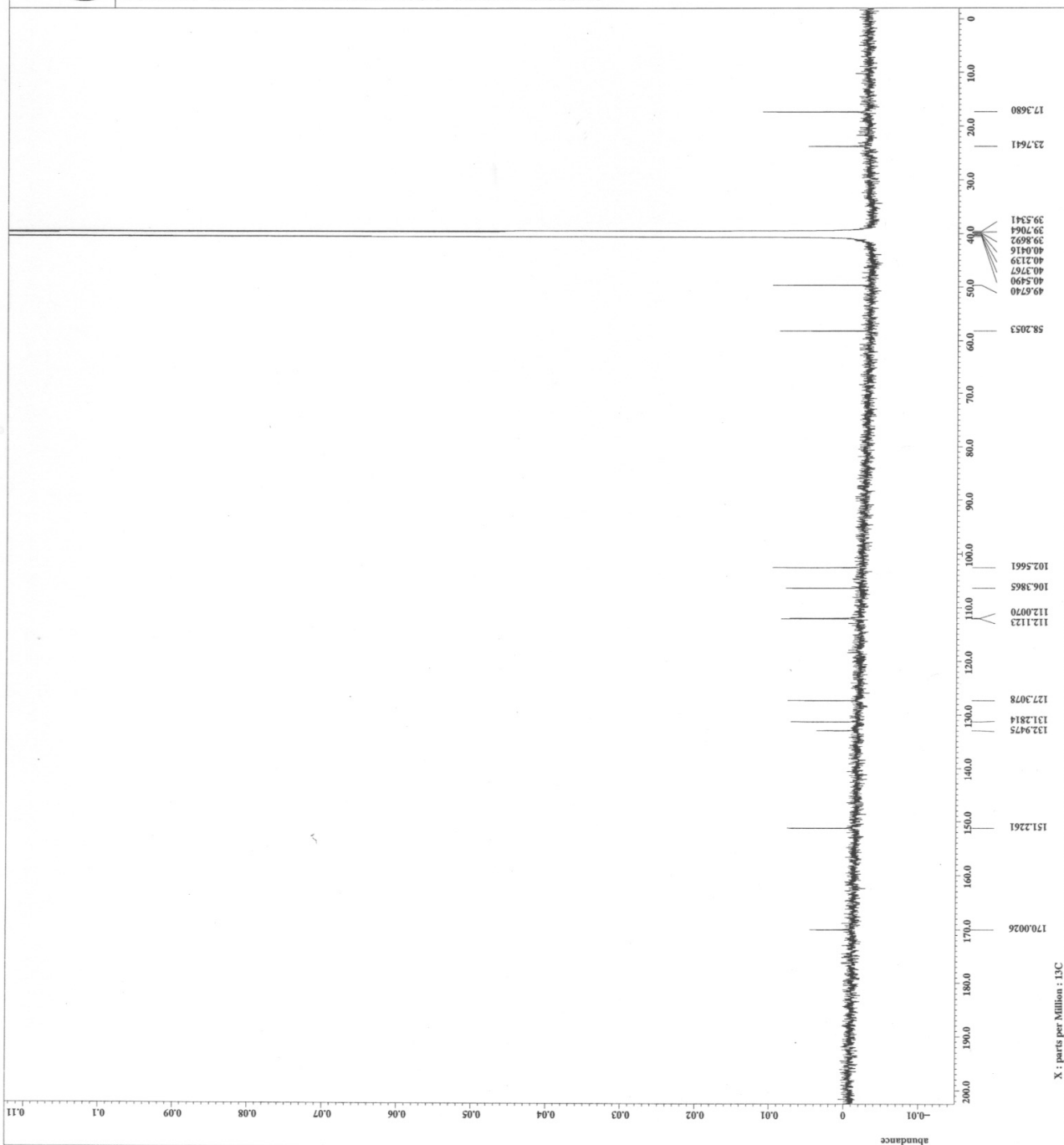
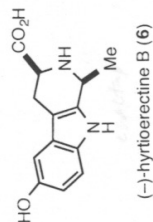


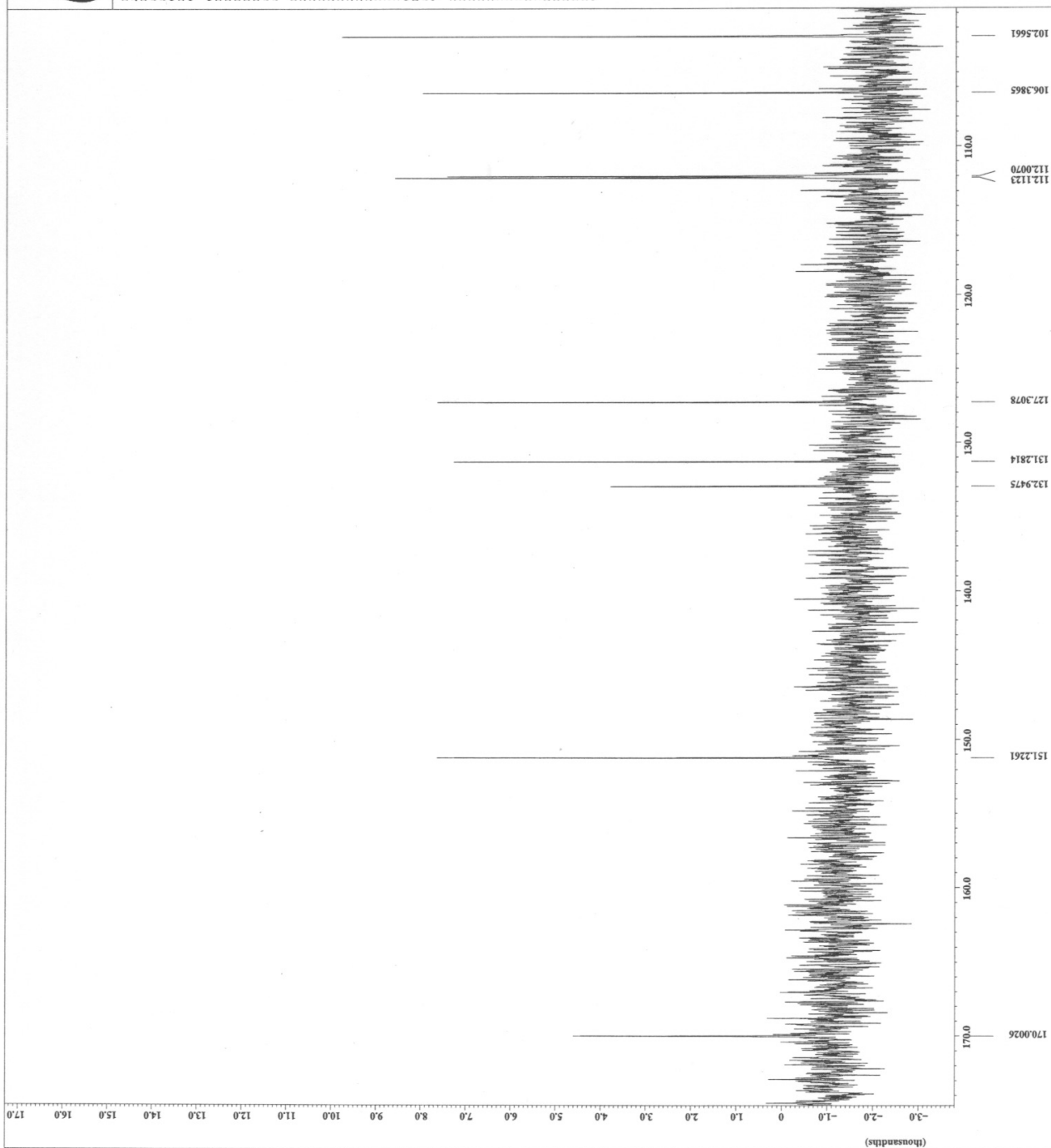
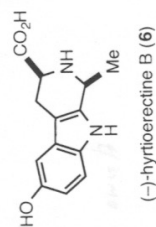




0.11

Filesname	B-11
Author	hydra
Experiment	single_pulse_dec
Sample	DMSP-D6
Solvent	DMSP-D6
Creation_time	10-DEC-2016 13:59:39
Creation_date	10-DEC-2016 13:59:39
Current_time	10-DEC-2016 14:09:29
Content	single_pulse decouple
data format	1D COMPLEX
Dma_line	26214
Dma_chan	13C
Dma_tune	13C
Dimensions	1
Site	ECA 500
Spectrometer	DMSP4L_NOR
field_strength	11.62936421 [T] (500IM
rotation	13
freq	134.9010055 [MHz]
q	134.9010055 [MHz]
offset	33748
q_resolution	1.1940925 [Hz]
ir_resolution	18.4625 [Hz]
ir_freq	495.13192398 [MHz]
ir_tune	FALSE
Glipped	1.00007
Mod_return	60007
Total_scan	36 (us)
X_90_dth	0.056018 [s]
X_90_tan	30 [deg]
X_angle	9.8 [deg]
X_tau	9.8 [dB]
ir_tau_dec	20.8 [333] [us]
ir_tau_dec	20.8 [dB]
ir_tau_dec	20.8 [dB]
Decoupling	TRUE
Initial_wait	1 [s]
Recv_gain	20
Recv_gain	60
Relaxation_delay	2.000000 [s]
Relaxation_time	2.000000 [s]
Temp_get	21.1 [deg]





X : parts per Million : 13C