

Amination/Cyclization Cascade by Acid-Catalyzed Activation of Indolenine for the One-Pot Synthesis of Phaitanthrin E

Supporting Information

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EXPERIMENTAL

1. General Methods

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 (δ) 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.).

2. Synthesis of 10a-f, S1

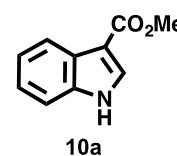
General Procedure A for Preparation of Substrate 10a-f:

According to Kozłowski's protocol,^{1,2} pyridine (1.2 mL, 14.2 mmol) was added to a mixture of indole (10.88 mmol) in THF (40 mL) at 0 °C and stirred for 0.5 h at 0 °C. A solution of trichloroacetyl chloride (1.6 mL, 14.2 mmol) in THF (30 mL) was added dropwise and the mixture was stirred at room temperature. After 16 h, the mixture was added to 10% HCl solution at 0 °C, extracted with AcOEt (300 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was dissolved in MeOH (150 mL), 10% KOH solution (20 mL) was added. Then, the mixture was heated to reflux for 5 h, followed by concentration under vacuum. The residue was diluted with AcOEt (200 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was purified by silica gel column chromatography with hexane/AcOEt (4/1) to give methyl carboxylate **10a-e**.

Methyl indole-3-carboxylate (10a).

Following the general procedure A from indole, **10a** (1.72 g, 90%) was obtained as an amorphous white powder.

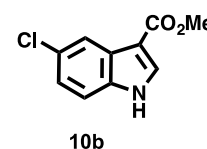
1.72 g, 90% yield, an amorphous white powder. Mp: 151-153 °C (EtOH). IR (CHCl₃): 3307, 3292, 1691 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ: 3.77 (s, 3H), 7.12-7.18 (m, 2H), 7.44 (dd, *J* = 1.7, 6.3 Hz, 1H), 7.96 (dd, *J* = 1.7, 6.3 Hz, 1H), 8.04 (d, *J* = 2.9 Hz, 1H), 11.89 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ: 51.1, 106.8, 112.9, 120.9, 121.8, 122.9, 126.2, 132.9, 136.9, 165.3. HR-ESI-MS *m/z*: Calcd for C₁₀H₉NO₂Na [(M+Na)⁺]: 198.0531. Found 198.0536.



Methyl 5-chloroindole-3-carboxylate (10b).

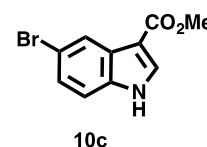
Following the general procedure A from 5-chloroindole, **10b** (1.64 g, 72%) was obtained as an amorphous white powder.

1.64 g, 72% yield, an amorphous white powder. Mp: 195-197 (CH₂Cl₂). IR (CHCl₃): 3275, 1697 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ: 3.78 (s, 3H), 7.19 (dd, *J* = 1.8, 8.6 Hz, 1H), 7.47 (d, *J* = 8.6 Hz, 1H), 7.92 (d, *J* = 1.7 Hz, 1H), 8.12 (d, *J* = 3.5 Hz, 1H), 12.09 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ: 51.3, 106.7, 114.6, 120.0, 122.9, 126.6, 127.3, 134.5, 135.4, 164.9. HR-ESI-MS *m/z*: Calcd for C₁₀H₈ClNNaO₂ [(M+Na)⁺]: 232.0141, 234.0112. Found 232.0152, 234.0120.



Methyl 5-bromoindole-3-carboxylate (10c).

Following the general procedure A from 5-bromoindole, **10c** (1.80 g, 65%) was obtained as an

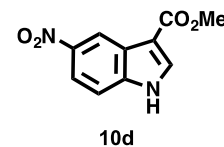


amorphous white powder.

1.80 g, 65% yield, n amorphous white powder. Mp: 215-217 (CH₂Cl₂). IR (CHCl₃): 3273, 3244, 1697 cm⁻¹. ¹H-NMR (CDCl₃) δ: 3.92 (s, 3H), 7.28 (d, *J* = 8.6 Hz, 1H), 7.36 (dd, *J* = 2.3, 8.6 Hz, 1H), 7.90 (d, *J* = 2.9 Hz, 1H), 8.32 (d, *J* = 1.8 Hz, 1H), 8.60 (br s, 1H). ¹³C-NMR (CDCl₃) δ: 51.3, 106.7, 114.6, 120.0, 122.9, 126.6, 127.3, 134.5, 135.4, 164.9. HR-ESI-MS *m/z*: Calcd for C₁₀H₈BrNNaO₂ [(M+Na)⁺]: 275.9636, 277.9616. Found 275.9628, 277.9618.

Methyl 5-nitroindole-3-carboxylate (10d).

Following the general procedure A from 5-nitroindole, **10d** (676 mg, 28%) was obtained as an amorphous white powder.

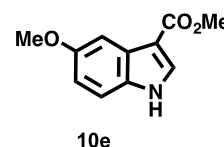


676 mg, 28% yield, an amorphous white powder. Mp: 270-273 (CH₂Cl₂). IR (CHCl₃): 3334, 1716 cm⁻¹.

¹H-NMR (DMSO-*d*₆) δ: 3.83 (s, 3H), 7.64 (d, *J* = 8.6 Hz, 1H), 8.07 (d, *J* = 9.6 Hz, 1H), 8.33 (s, 1H), 8.82 (s, 1H), 12.53 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ: 51.7, 108.9, 113.7, 117.4, 118.3, 125.5, 136.7, 140.1, 142.9, 164.5. HR-ESI-MS *m/z*: Calcd for C₁₀H₈N₂O₄ [M⁺]: 220.0484. Found 220.0490.

Methyl 5-methoxyindole-3-carboxylate (10e).

Following the general procedure A from 5-methoxyindole, **10e** (1.88 g, 84%) was obtained as an amorphous white powder.



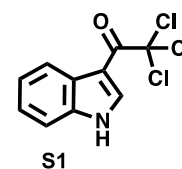
1.88 g, 84% yield, an amorphous white powder. Mp: 140-142 (CH₂Cl₂/hexane). IR (CHCl₃): 3290, 3275, 1689 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ: 3.75 (s, 3H), 3.76 (s, 3H), 6.80 (dd, *J* = 2.3, 9.2 Hz, 1H), 7.33 (d, *J* = 8.6 Hz, 1H), 7.44 (d, *J* = 2.9 Hz, 1H), 7.97 (d, *J* = 3.4 Hz, 1H), 11.76 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ: 51.1, 55.8, 102.6, 106.5, 112.9, 113.6, 127.0, 131.8, 133.0, 155.5, 165.3. HR-ESI-MS *m/z*: Calcd for C₁₁H₁₁NNaO₃ [(M+Na)⁺]: 228.0637. Found 228.0635.

Procedure for Preparation of Ethyl Ester Precursor S1:

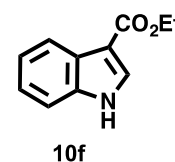
According to Kozlowski's protocol,^{1,2} pyridine (0.6 mL, 7.1 mmol) was added to a mixture of indole (5.44 mmol) in THF (20 mL) at 0 °C and stirred for 0.5 h at 0 °C. A solution of trichloroacetyl chloride (0.8 mL, 7.1 mmol) in THF (15 mL) was added dropwise and the mixture was stirred at room temperature. After 16 h, the mixture was added to 10% HCl solution at 0 °C, extracted with AcOEt (200 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was purified by silica gel column chromatography with hexane/AcOEt (3/1) to give **S1** (1.27 g, 89%) as an amorphous white powder.

2,2,2-Trichloro-1-(1*H*-indol-3-yl)ethan-1-one (S1).

1.27 g, 89% yield, an amorphous white powder. Mp: 224-226 (CH₂Cl₂). IR (CHCl₃): 3275, 3253, 1672 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ: 7.26-7.29 (m, 2H), 7.54 (dd, *J* = 3.1, 6.1 Hz, 1H), 8.15 (dd, *J* = 3.1, 5.4 Hz, 1H), 8.55 (s, 1H), 12.50 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ: 97.0, 105.3, 113.4, 121.7, 123.6, 124.3, 127.6, 136.6, 137.2, 177.3. HR-ESI-MS *m/z*: Calcd for C₁₀H₇Cl₃NO [(M+H)⁺]: 261.9593, 263.9564, 265.9534. Found 261.9600, 263.9569, 265.9531.



Ethyl indole-3-carboxylate (10f).



10% KOH solution (5 mL) was added to a solution of S1 (788 mg, 3 mmol) in EtOH (40 mL) and the mixture was heated to reflux for 16 h, followed by concentration under vacuum. The residue was diluted 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 hexane/AcOEt (4/1) to give ethyl carboxylate **10f** (433 mg, 76%) as an amorphous white powder.

433 mg, 76% yield, an amorphous white powder. Mp: 125-127 °C (EtOH). IR (CHCl₃): 3307, 3275, 1681 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ: 1.29 (t, *J* = 6.9 Hz, 3H), 4.23 (dd, *J* = 7.5, 14.3 Hz, 2H), 7.13-7.18 (m, 2H), 7.44 (dd, *J* = 1.7, 6.9 Hz, 1H), 7.97 (dd, *J* = 1.8, 8.6 Hz, 1H), 8.03 (d, *J* = 2.3 Hz, 1H), 11.88 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ: 15.0, 59.5, 107.2, 112.9, 121.0, 121.7, 122.8, 126.2, 132.9, 136.9, 164.9. HR-ESI-MS *m/z*: Calcd for C₁₁H₁₁N₂NaO₂ [(M+Na)⁺]: 212.0687. Found 212.0680.

3. Optimization of Reaction Conditions (Table 1).

Typical procedure 1 (entries 1-6): NCS (147 mg, 1.1 mmol) was added to a solution of **10a** (175 mg, 1 mmol) and Et₃N (0.28 mL, 2 mmol) in CH₂Cl₂ (10 mL) at room temperature, and the mixture was stirred at room temperature. After 0.5 h, anthranilic acid methyl ester **11a** (302 mg, 2 mmol) and acid (0.1 mmol) in CH₂Cl₂ (2 mL) was dropwise added to the reaction mixtures and the mixture was stirred at room temperature. After 2 h, the mixture was added to 10% NaOH 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 hexane/AcOEt (3/1) to give **5aa**.

Typical procedure 2 (entries 7-9): Electrophile (1.1 mmol) was added to a solution of **10a** (175 mg, 1 mmol) and Et₃N (0.28 mL, 2 mmol) in CH₂Cl₂ (10 mL) at room temperature, and the mixture was stirred at room temperature. After 0.5 h, anthranilic acid methyl ester **11a** (302 mg, 2 mmol) and trifluoroacetic acid (8 μL, 0.1 mmol) in CH₂Cl₂ (2 mL) was dropwise added to the reaction mixtures and the mixture was stirred at room temperature. After 2 h, the mixture was added to saturated Na₂S₂O₃ solution at 0 °C, and vigorously stirred at 0 °C. After 0.5 h, the mixture was 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 hexane/AcOEt (3/1).

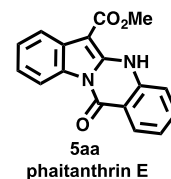
Typical procedure 3 (entries 10-17): NCS (147 mg, 1.1 mmol) was added to a solution of **10a** (175 mg, 1 mmol) and base (2 mmol) in CH₂Cl₂ (10 mL) at room temperature, and the mixture was stirred at room temperature. After 0.5 h, anthranilic acid methyl ester **11a** (302 mg, 2 mmol) and trifluoroacetic acid (8 μL, 0.1 mmol) in CH₂Cl₂ (2 mL) was dropwise added to the reaction mixtures and the mixture was stirred at room temperature. After 2 h, the mixture was added to 10% NaOH 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 hexane/AcOEt (3/1) to give **5aa**.

4. Synthesis of 5 (Scheme 2).

Typical procedure A: NCS (441 mg, 3.3 mmol) was added to a solution of **10a** (526 mg, 3 mmol) and Et₃N (0.84 mL, 6 mmol) in CH₂Cl₂ (25 mL) at room temperature, and the mixture was stirred at room temperature. After 0.5 h, anthranilic acid methyl ester **11a** (907 mg, 6 mmol) and trifluoroacetic acid (22 μ L, 0.3 mmol) in CH₂Cl₂ (5 mL) was dropwise added to the reaction mixtures and the mixture was stirred at room temperature. After 2 h, the mixture was added to 10% NaOH solution at 0 °C, extracted with AcOEt (150 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was purified by silica gel column chromatography with hexane/AcOEt (3/1) to give phaitanthrin E **5aa** (791 mg, 90% yield).

Phaitanthrin E (**5aa**).³⁻⁴

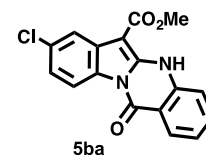
791 mg, 90% yield, an amorphous white powder. Mp: 214-216 °C (EtOH). IR (CHCl₃): 3329, 1697, 1665, 1626, 1579 cm⁻¹. ¹H-NMR (CDCl₃) δ : 4.01 (s, 3H), 7.28 (d, J = 8.6 Hz, 1H), 7.30-7.34 (m, 2H), 7.43 (td, J = 1.2, 8.0 Hz, 1H), 7.71 (td, J = 1.7, 7.7 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 8.39 (d, J = 8.0 Hz, 1H), 8.70 (d, J = 8.0 Hz, 1H), 10.29 (br s, 1H). ¹³C-NMR (CDCl₃) δ : 51.4, 86.7, 114.4, 115.7, 116.3, 119.4, 122.4, 123.2, 125.7, 126.3, 128.7, 130.4, 135.3, 138.2, 144.1, 158.5, 167.3. HR-ESI-MS m/z : Calcd for C₁₇H₁₃N₂O₃ [(M+H)⁺]: 293.0926. Found 293.0926.



Methyl 8-chloro-12-oxo-5,12-dihydroindolo[2,1-b]quinazoline-6-carboxylate (**5ba**).

According to the typical procedure A, **5ba** (258 mg, 26% yield) was obtained as an amorphous white powder.

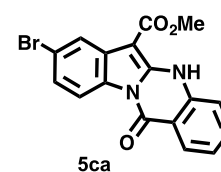
258 mg, 26% yield, an amorphous white powder. Mp: 286-289 °C (EtOH). IR (CHCl₃): 3332, 1697, 1662, 1620, 1577 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 3.91 (s, 3H), 7.28 (dd, J = 2.3, 8.6 Hz, 1H), 7.35 (t, J = 8.0 Hz, 1H), 7.79 (td, J = 1.8, 7.7 Hz, 1H), 7.89 (d, J = 2.3 Hz, 1H), 8.00 (d, J = 8.6 Hz, 1H), 8.20 (dd, J = 1.2, 8.0 Hz, 1H), 8.58 (d, J = 8.6 Hz, 1H), 11.47 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 51.4, 86.1, 114.1, 117.5, 118.3, 118.6, 121.7, 123.5, 127.7, 128.7, 129.2, 130.4, 135.7, 140.0, 144.7, 158.8, 164.9. HR-ESI-MS m/z : Calcd for C₁₇H₁₂ClN₂O₃ [(M+H)⁺]: 327.0536, 329.0507. Found 327.0545, 329.0516.



Methyl 8-bromo-12-oxo-5,12-dihydroindolo[2,1-b]quinazoline-6-carboxylate (**5ca**).

According to the typical procedure A, **5ca** (89 mg, 8% yield) was obtained as an amorphous pale yellow powder.

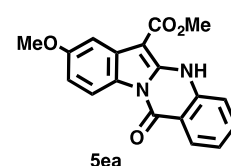
89 mg, 8% yield, an amorphous pale yellow powder. Mp: 303-306 °C (EtOH). IR (CHCl₃): 3462, 1689 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 3.91 (s, 3H), 7.34 (t, J = 7.5 Hz, 1H), 7.41 (dd, J = 2.3, 9.2 Hz, 1H), 7.79 (t, J = 9.2 Hz, 1H), 7.97 (t, J = 7.4 Hz, 1H), 8.00 (d, J = 8.6 Hz, 1H), 8.03 (d, J = 1.7 Hz, 1H), 8.20 (d, J = 8.0 Hz, 1H), 8.53 (d, J = 8.6 Hz, 1H), 11.47 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ : 51.4, 85.9, 114.1, 117.8, 118.4, 118.6, 121.5, 123.4, 124.3, 127.5, 129.1, 129.6, 134.6, 135.6, 144.7, 158.9, 164.9. HR-ESI-MS m/z : Calcd for C₁₇H₁₁BrN₂O₃ [M⁺]: 369.9953, 371.9933. Found 369.9951, 371.9937.



Methyl 8-methoxy-12-oxo-5,12-dihydroindolo[2,1-b]quinazoline-6-carboxylate (**5ea**).

According to the typical procedure A, **5ea** (724 mg, 75% yield) was obtained as an amorphous white powder.

724 mg, 75% yield, an amorphous white powder. Mp: 234-235 °C (EtOH). IR (CHCl₃): 3325, 1689, 1625, 1579, 1529 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ : 3.82 (s, 3H), 3.91 (s, 3H), 6.84 (d, J = 9.2 Hz, 1H), 7.33 (t, J = 7.5 Hz, 1H), 7.46 (s, 1H), 7.77 (t, J = 8.0 Hz, 1H), 7.95 (d, J = 8.6 Hz, 1H), 8.20 (d, J = 8.0 Hz, 1H), 8.49 (d, J = 8.6



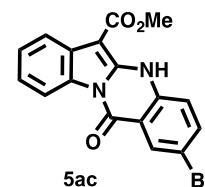
Hz, 1H), 11.26 (br s, 1H). ^{13}C -NMR (DMSO- d_6) δ : 51.3, 55.9, 86.4, 103.4, 109.5, 113.9, 116.9, 118.0, 123.2, 124.6, 127.5, 128.8, 135.3, 139.7, 144.0, 158.0, 158.5, 165.2. HR-ESI-MS m/z : Calcd for $\text{C}_{18}\text{H}_{14}\text{N}_2\text{NaO}_3$ $[(\text{M}+\text{Na})^+]$: 345.0851. Found 345.0851.

Methyl

2-bromo-12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (**5ac**).

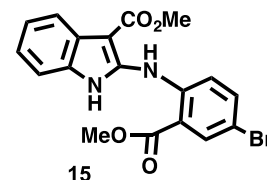
According to the typical procedure A, **5ac** (92 mg, 8% yield) and **15** (849 mg, 70% yield) were obtained.

5ac: 92 mg, 8% yield, yellow solids. Mp: 240-242 °C (EtOH). IR (CHCl₃): 3325, 1730, 1697, 1625 cm^{-1} . ^1H -NMR (DMSO- d_6) δ : 3.91 (s, 3H), 7.28 (t, J = 6.9 Hz, 1H), 7.41 (t, J = 8.0 Hz, 1H), 7.93 (dd, J = 2.3, 9.2 Hz, 1H), 7.97 (t, J = 9.2 Hz, 2H), 8.25 (d, J = 1.7 Hz, 1H), 8.59 (d, J = 8.1 Hz, 1H), 11.50 (br s, 1H). ^{13}C -NMR (DMSO- d_6) δ : 51.5, 86.8, 114.7, 115.8, 116.1, 119.6, 120.4, 122.3, 125.9, 127.2, 129.4, 130.1, 138.0, 138.9, 143.4, 157.9, 165.2. HR-ESI-MS m/z : Calcd for $\text{C}_{17}\text{H}_{11}\text{BrN}_2\text{O}_3$ $[\text{M}^+]$: 369.9953, 371.9933. Found 369.9949, 371.9935.



Methyl 2-((4-bromo-2-(methoxycarbonyl)phenyl)amino)-1H-indole-3-carboxylate (**15**).

849 mg, 70% yield, amorphous pale yellow powder. Mp: 234-236 °C (EtOH). IR (CHCl₃): 3446, 1668, 1583 cm^{-1} . ^1H -NMR (CDCl₃) δ : 3.96 (s, 3H), 3.98 (s, 3H), 7.12 (t, J = 7.5 Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H), 7.22 (d, J = 7.5 Hz, 1H), 7.49 (d, J = 8.6 Hz, 1H), 7.63 (dd, J = 1.7, 8.6 Hz, 1H), 7.90 (d, J = 7.5 Hz, 1H), 8.18 (d, J = 2.3 Hz, 1H), 8.38 (br s, 1H), 11.27 (br s, 1H). ^{13}C -NMR (CDCl₃) δ : 51.1, 52.8, 90.7, 110.2, 113.3, 118.0, 118.6, 120.1, 121.7, 122.4, 126.1, 131.6, 135.2, 137.3, 141.0, 145.1, 166.2, 166.8. HR-ESI-MS m/z : Calcd for $\text{C}_{18}\text{H}_{15}\text{BrN}_2\text{NaO}_4$ $[(\text{M}+\text{Na})^+]$: 425.0113, 427.0092. Found 425.0111, 427.0098.

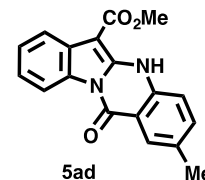


Typical Procedure B: NCS (3.3 mmol) was added to a solution of **5a** (3 mmol) and Et₃N (0.84 mL, 6 mmol) in CH₂Cl₂ (25 mL) at room temperature, and the mixture was stirred at room temperature. After 0.5 h, 5-bromoanthranilic acid methyl ester **11c** (1.38 g, 6 mmol) and trifluoroacetic acid (22 μL , 0.3 mmol) in CH₂Cl₂ (10 mL) was dropwise added to the reaction mixtures and the mixture was stirred at room temperature. After 72 h, K₂CO₃ (829 mg, 6 mmol) was portionwise added to the mixture at room temperature, and stirred at room temperature. After 16 h, the mixture was added to H₂O at 0 °C, extracted with AcOEt (150 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was purified by silica gel column chromatography with hexane/AcOEt (3/1) to give **5ac** (715 mg, 64% yield).

Methyl 2-methyl-12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (**5ad**).

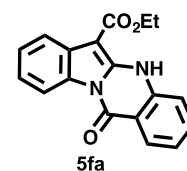
According to the typical procedure A, **5ad** (698 mg, 76% yield) was obtained as an amorphous white powder.

698 mg, 76% yield, an amorphous white powder. Mp: 216-218 °C (EtOH). IR (CHCl₃): 3332, 1697, 1662, 1620, 1577 cm^{-1} . ^1H -NMR (CDCl₃) δ : 2.47 (s, 3H), 4.01 (s, 3H), 7.19 (d, J = 8.0 Hz, 1H), 7.31 (td, J = 1.2, 8.1 Hz, 1H), 7.43 (t, J = 7.5 Hz, 1H), 7.53 (dd, J = 1.2, 8.0 Hz, 1H), 7.95 (d, J = 7.5 Hz, 1H), 8.19 (s, 1H), 8.69 (d, J = 8.6 Hz, 1H), 10.25 (br s, 1H). ^{13}C -NMR (CDCl₃) δ : 20.9, 51.3, 86.3, 114.2, 115.6, 116.3, 119.4, 122.3, 125.7, 126.4, 128.1, 130.4, 133.1, 136.1, 136.6, 144.3, 158.6, 167.4. HR-ESI-MS m/z : Calcd for $\text{C}_{18}\text{H}_{14}\text{N}_2\text{O}_3$ $[\text{M}^+]$: 306.1004. Found 306.1005.



Ethyl 12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (**5fa**).³

According to the typical procedure A, **5fa** (845 mg, 92% yield) was obtained as an amorphous white powder.

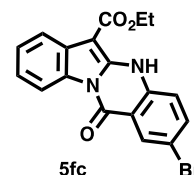


845 mg, 92% yield, an amorphous white powder. Mp: 182-183 °C (EtOH). IR (CHCl₃): 3327, 1697, 1660, 1625, 1579 cm⁻¹. ¹H-NMR (CDCl₃) δ: 1.51 (t, *J* = 6.9 Hz, 3H), 4.47 (dd, *J* = 6.9, 14.3 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.71 (t, *J* = 8.6 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.71 (d, *J* = 8.0 Hz, 1H), 10.32 (br s, 1H). ¹³C-NMR (CDCl₃) δ: 14.7, 60.3, 86.9, 114.3, 115.7, 116.3, 119.5, 122.4, 123.1, 125.7, 126.4, 128.7, 130.4, 135.3, 138.2, 144.1, 158.6, 167.1. HR-ESI-MS *m/z*: Calcd for C₁₈H₁₄N₂NaO₃ [(M+Na)⁺]: 329.0902. Found 329.0898.

Ethyl 2-bromo-12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (**5fc**).

According to the typical procedure B, **5fc** (858 mg, 74% yield) was obtained as yellow solids.

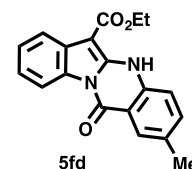
858 mg, 74% yield, yellow solids. Mp: 320-323 °C (EtOH). IR (CHCl₃): 3365, 1670, 1625 cm⁻¹. ¹H-NMR (CDCl₃) δ: 1.50 (t, *J* = 6.9 Hz, 3H), 4.48 (dd, *J* = 6.9, 14.3 Hz, 2H), 7.18 (d, *J* = 9.2 Hz, 1H), 7.34 (td, *J* = 1.2, 8.6 Hz, 1H), 7.45 (td, *J* = 1.2, 7.5 Hz, 1H), 7.79 (dd, *J* = 2.3, 8.6 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 8.51 (d, *J* = 2.3 Hz, 1H), 8.69 (d, *J* = 8.0 Hz, 1H), 10.36 (br s, 1H). ¹³C-NMR (CDCl₃) δ: 14.7, 60.5, 87.4, 115.6, 115.7, 116.3, 117.4, 119.6, 122.7, 125.9, 126.4, 130.3, 131.2, 137.1, 138.2, 143.6, 157.3, 167.0. HR-ESI-MS *m/z*: Calcd for C₁₈H₁₃BrN₂NaO₃ [(M+Na)⁺]: 385.0188, 387.0167. Found 385.0190, 387.0171.



Ethyl 2-methyl-12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (**5fd**).

According to the typical procedure A, **5fd** (768 mg, 80% yield) was obtained as pale yellow solids.

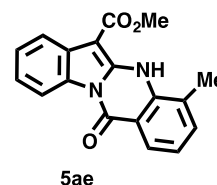
768 mg, 80% yield, pale yellow solids. Mp: 194-195 °C (EtOH). IR (CHCl₃): 3329, 1691, 1658, 1620, 1577 cm⁻¹. ¹H-NMR (CDCl₃) δ: 1.50 (t, *J* = 6.9 Hz, 3H), 2.46 (s, 3H), 4.46 (dd, *J* = 7.4, 14.4 Hz, 2H), 7.16 (d, *J* = 8.6 Hz, 1H), 7.30 (td, *J* = 1.2, 6.9 Hz, 1H), 7.42 (td, *J* = 1.1, 6.9 Hz, 1H), 7.51 (dd, *J* = 1.8, 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 8.16 (s, 1H), 8.70 (d, *J* = 8.6 Hz, 1H), 10.25 (br s, 1H). ¹³C-NMR (CDCl₃) δ: 14.7, 20.9, 60.2, 86.5, 114.1, 115.6, 116.3, 119.4, 122.2, 125.6, 126.5, 128.1, 130.4, 133.0, 136.1, 136.5, 144.2, 158.6, 167.1. HR-ESI-MS *m/z*: Calcd for C₁₉H₁₆N₂NaO₃ [(M+Na)⁺]: 343.1059 Found 343.1062.



Methyl 4-methyl-12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (**5ae**).

According to the typical procedure A, **5ae** (476 mg, 52% yield) was obtained as an amorphous pale yellow powder.

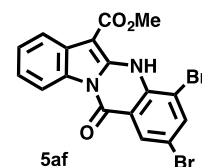
476 mg, 52% yield, an amorphous pale yellow powder. Mp: 220-222 °C (EtOH). IR (CHCl₃): 3446, 3334, 1697, 1624 cm⁻¹. ¹H-NMR (CDCl₃) δ: 2.55 (s, 3H), 4.02 (s, 3H), 7.23 (t, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.1 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 7.4 Hz, 1H), 7.93 (d, *J* = 6.3 Hz, 1H), 8.25 (d, *J* = 8.0 Hz, 1H), 8.70 (d, *J* = 8.1 Hz, 1H), 10.41 (br s, 1H). ¹³C-NMR (CDCl₃) δ: 16.4, 51.4, 86.8, 114.2, 116.3, 119.4, 122.4, 122.7, 123.3, 125.7, 126.5, 130.3, 135.9, 136.9, 144.2, 158.8, 167.7. HR-ESI-MS *m/z*: Calcd for C₁₈H₁₅N₂O₃ [(M+H)⁺]: 307.1083. Found 307.1077.



Methyl 2,4-dibromo-12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (**5af**).

According to the typical procedure B, **5af** (208 mg, 15% yield) was obtained as yellow solids.

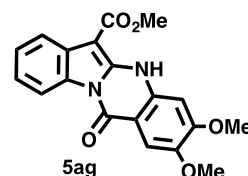
208 mg, 15% yield, yellow solids. Mp: 235-238 °C (EtOH). IR (CHCl₃): 3367, 1697, 1604, 1570, 1535 cm⁻¹. ¹H-NMR (CDCl₃) δ: 4.05 (s, 3H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.99 (m, 1H), 8.05 (s, 1H), 8.49 (s, 1H), 8.66 (d, *J* = 8.0 Hz, 1H), 10.81 (br s, 1H). ¹³C-NMR (CDCl₃) δ: 51.7, 88.3, 110.3, 114.9, 116.2, 116.3, 119.8, 123.1, 126.2, 130.2, 130.7, 135.5, 140.0, 142.7, 156.5, 167.1 (one sp² signal was not observed because of overlapping). HR-ESI-MS *m/z*: Calcd for C₁₇H₁₀Br₂N₂NaO₃ [(M+Na)⁺]: 470.8956, 472.8935, 474.8915. Found 470.8953, 472.8953, 474.8930.



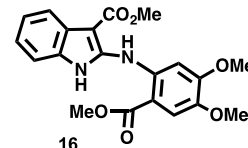
Methyl 2,3-dimethoxy-12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (5ag).

According to the typical procedure A, **5ag** (255 mg, 24% yield) and **16** (496 mg, 43% yield) were obtained.

5ag: 255 mg, 24% yield, an amorphous white powder. Mp: 210-212 °C (EtOH). IR (CHCl₃): 3332, 1681, 1658, 1629, 1616 cm⁻¹. ¹H-NMR (CDCl₃) δ: 3.97 (s, 3H), 3.99 (s, 3H), 4.00 (s, 3H), 6.66 (s, 1H), 7.30 (t, *J* = 8.1 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.69 (s, 1H), 7.93 (d, *J* = 7.5 Hz, 1H), 8.69 (d, *J* = 8.0 Hz, 1H), 10.23 (br s, 1H). ¹³C-NMR (CDCl₃) δ: 51.3, 56.4, 56.5, 86.1, 97.5, 106.7, 107.9, 116.2, 119.3, 122.1, 125.5, 126.2, 130.2, 134.2, 144.2, 146.3, 155.9, 158.2, 167.4. HR-ESI-MS *m/z*: Calcd for C₁₉H₁₇N₂O₅ [(M+H)⁺]: 353.1137. Found 353.1141.

**Methyl 2-((4,5-dimethoxy-2-(methoxycarbonyl)phenyl)amino)-1*H*-indole-3-carboxylate (16).**

496 mg, 43% yield, an amorphous white powder. Mp: 224-226 °C (EtOH). IR (CHCl₃): 3446, 1670, 1593, 1566 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ: 3.78 (s, 3H), 3.81 (s, 3H), 3.83 (s, 3H), 3.88 (s, 3H), 6.98 (td, *J* = 1.2, 7.5 Hz, 1H), 7.03 (td, *J* = 1.2, 8.0 Hz, 1H), 7.17 (s, 1H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.42 (s, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 10.73 (br s, 1H), 11.65 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ: 50.9, 52.6, 56.1, 56.4, 88.3, 103.2, 108.6, 111.5, 113.5, 119.2, 121.1, 121.7, 126.3, 133.3, 136.9, 143.9, 146.8, 154.3, 166.2, 166.9. HR-ESI-MS *m/z*: Calcd for C₂₀H₂₀N₂NaO₆ [(M+Na)⁺]: 407.1219. Found 407.1220.

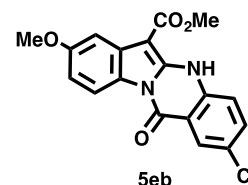


According to the typical procedure B, **5ag** (592 mg, 56% yield) was obtained.

Methyl 2-chloro-8-methoxy-12-oxo-5,12-dihydroindolo[2,1-*b*]quinazoline-6-carboxylate (5eb).

According to the typical procedure A, **5eb** (666 mg, 62% yield) was obtained as an amorphous white powder.

666 mg, 62% yield, an amorphous white powder. Mp: 234-235 °C (EtOH). IR (CHCl₃): 3325, 1689, 1625, 1579, 1529 cm⁻¹. ¹H-NMR (DMSO-*d*₆) δ: 3.78 (s, 3H), 3.87 (s, 3H), 6.78 (d, *J* = 8.6 Hz, 1H), 7.39 (s, 1H), 7.75 (d, *J* = 9.2 Hz, 1H), 7.93 (d, *J* = 9.2 Hz, 1H), 8.05 (s, 1H), 8.40 (d, *J* = 9.2 Hz, 1H), 11.39 (br s, 1H). ¹³C-NMR (DMSO-*d*₆) δ: 51.2, 55.9, 86.7, 103.4, 109.3, 115.2, 116.8, 121.0, 124.4, 126.2, 126.6, 129.2, 134.8, 139.6, 144.4, 157.6, 158.1, 165.1. HR-ESI-MS *m/z*: Calcd for C₁₈H₁₄ClN₂O₄ [(M+NH)⁺]: 357.0642. Found 359.0613.



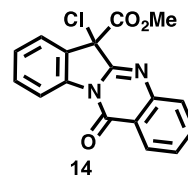
5. Synthesis of 14 (Scheme 3c)

NCS (134 mg, 1.1 mmol) was added to a solution of **5aa** (292 mg, 1 mmol) in CH₂Cl₂ (10 mL) at room temperature, and the mixture was stirred at room temperature. After 0.5 h, the mixture was added to 10% NaOH 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 hexane/AcOEt (3/1) to give **14** (287 mg, 88% yield) as white solids.

Methyl 6-chloro-12-oxo-6,12-dihydroindolo[2,1-b]quinazoline-6-carboxylate (**14**).

287 mg, 88% yield, white solids. Mp: 188-191 °C (CH₂Cl₂). IR (CHCl₃): 1764,

¹H-NMR (acetone-*d*₆) δ: 3.65 (s, 3H), 6.36 (br s, 1H), 7.24 (dt, *J* = 1.1, 7.4 Hz, 8.0 Hz, 1H), 7.61 (dd, *J* = 1.2, 7.5 Hz, 1H), 7.63 (dt, *J* = 1.7, 7.8 Hz, 1H), 7.75 (d, (dt, *J* = 1.7, 7.5 Hz, 1H), 8.35 (dd, *J* = 1.2, 8.0 Hz, 1H), 8.52 (dd, *J* = 1.2, 8.0 Hz, (acetone-*d*₆) δ: 52.9, 79.4, 116.8, 122.1, 124.1, 126.8, 127.0, 127.9, 128.0, 130.6, 147.3, 157.9, 158.9, 169.7. HR-ESI-MS *m/z*: Calcd for C₁₇H₁₂ClN₂O₃ [(M+H)⁺]: 327.0536, 329.0507. Found 327.0536, 329.0515.



1689, 1647, 1600 cm⁻¹.
1H), 7.59 (dd, *J* = 1.2, *J* = 7.4 Hz, 1H), 7.88 (1H). ¹³C-NMR, 131.0, 134.8, 140.2,

6. Cyclization of 15 (Scheme 3d)

K₂CO₃ (138 mg, 1 mmol) was added to a solution of **15** (202 mg, 0.5 mmol) in MeCN (10 mL) at room temperature, and the mixture was stirred at room temperature. After 2 h, the mixture was added to H₂O 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 hexane/AcOEt (3/1) to give **5ac** (167 mg, 90% yield).

Cyclization of 16 (Scheme 3d)

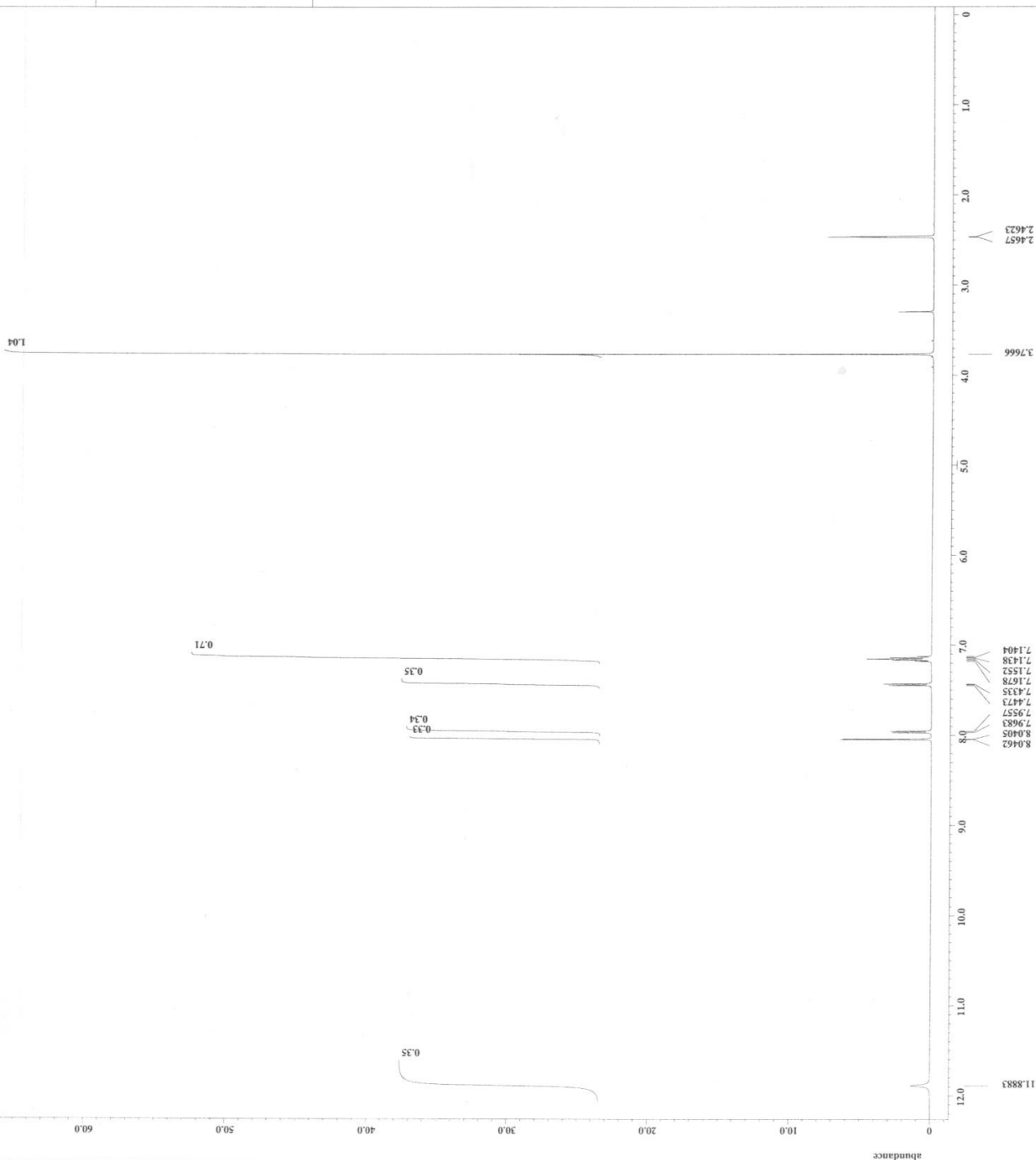
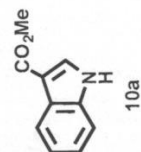
K₂CO₃ (138 mg, 1 mmol) was added to a solution of **16** (192 mg, 0.5 mmol) in MeCN (10 mL) at room temperature, and the mixture was stirred at room temperature. After 2 h, the mixture was added to H₂O at 0 °C, extracted with AcOEt (100 mL), washed with brine, and dried over MgSO₄. The solvent was removed, and the residue was purified by silica gel column chromatography with hexane/AcOEt (3/1) to give **5ag** (147 mg, 83% yield).

7. References

- (1) Linton, E. C.; Kozlowski, M. C. *J. Am. Chem. Soc.* **2008**, *130*, 16162.
- (2) Lu, W.-J.; Switalska, M.; Wang, L.; Yonezawa, M.; El-Sayed, I. E.; Wietrzyk, J.; Inokuchi, T. *Med. Chem. Res.* **2013**, *22*, 4492.
- (3) Vaidya, S. D.; Argade, N. P. *Org. Lett.* **2015**, *17*, 6218.
- (4) Vaidya, S. D.; Argade, N. P. *Synthesis* **2016**, *48*, 2896.

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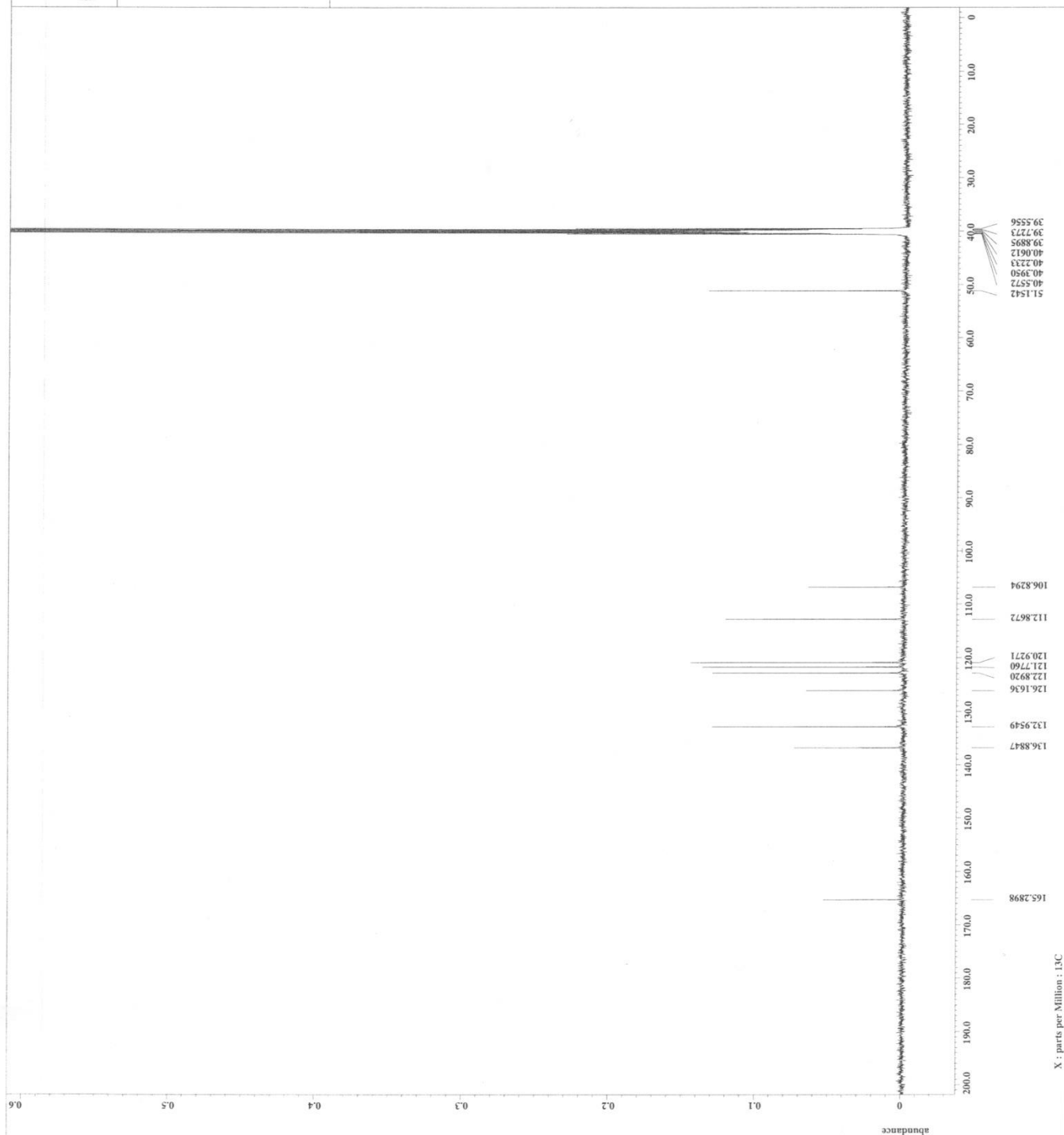
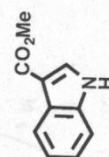
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ppm
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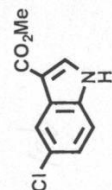
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Derived from: TA160324-1.jdf

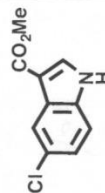
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10b

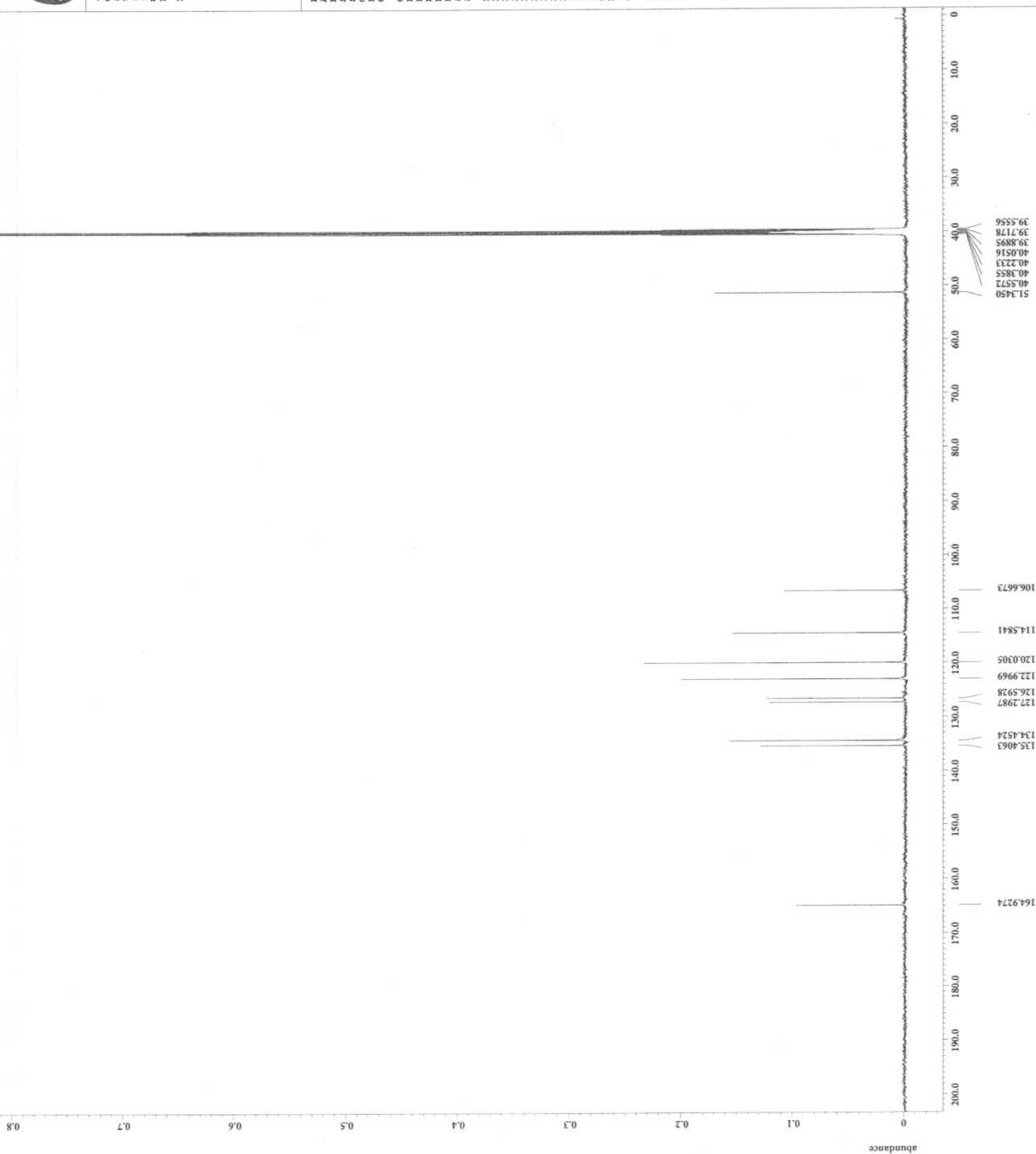
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10b

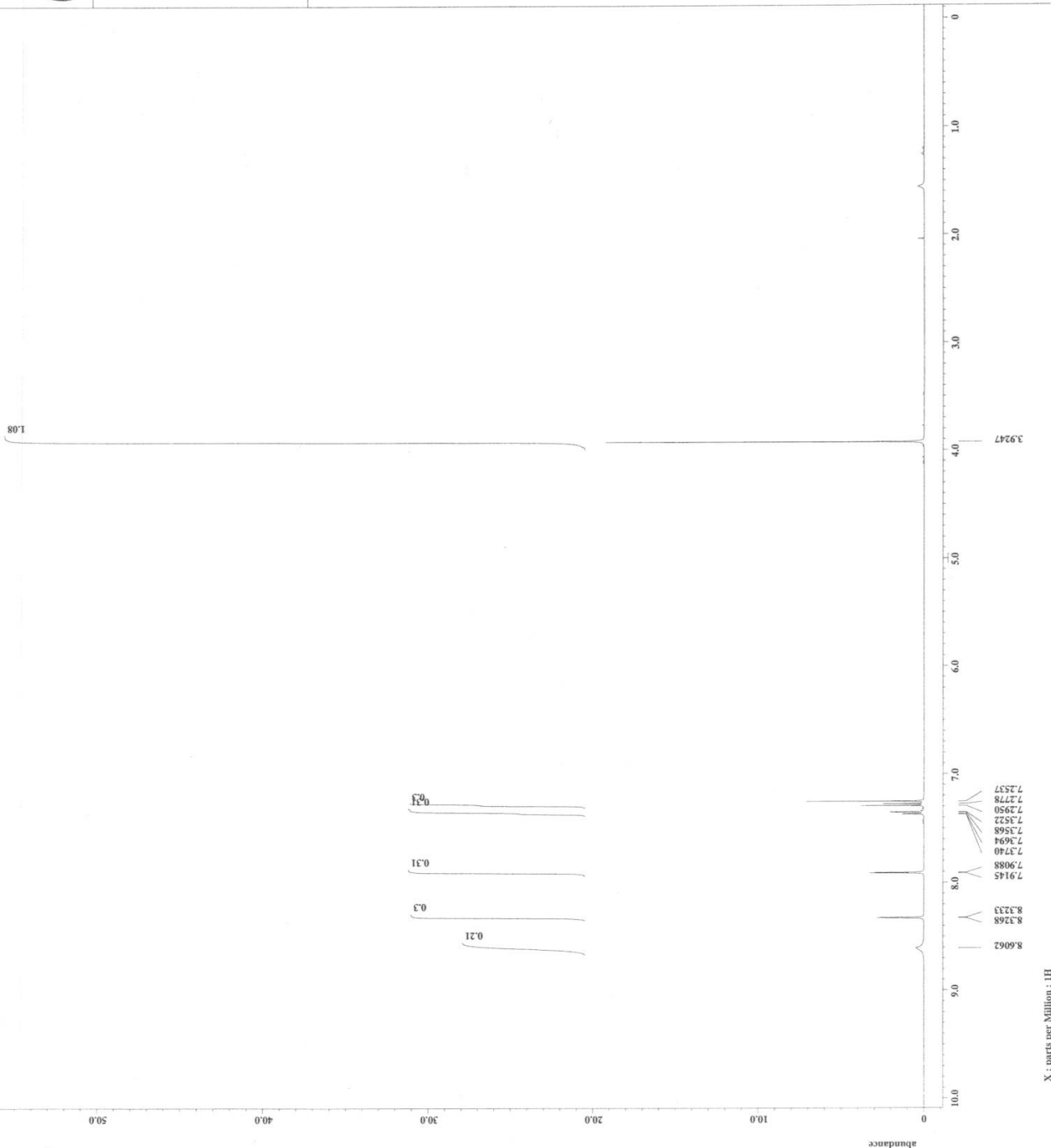
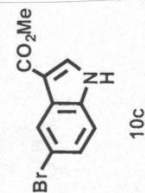


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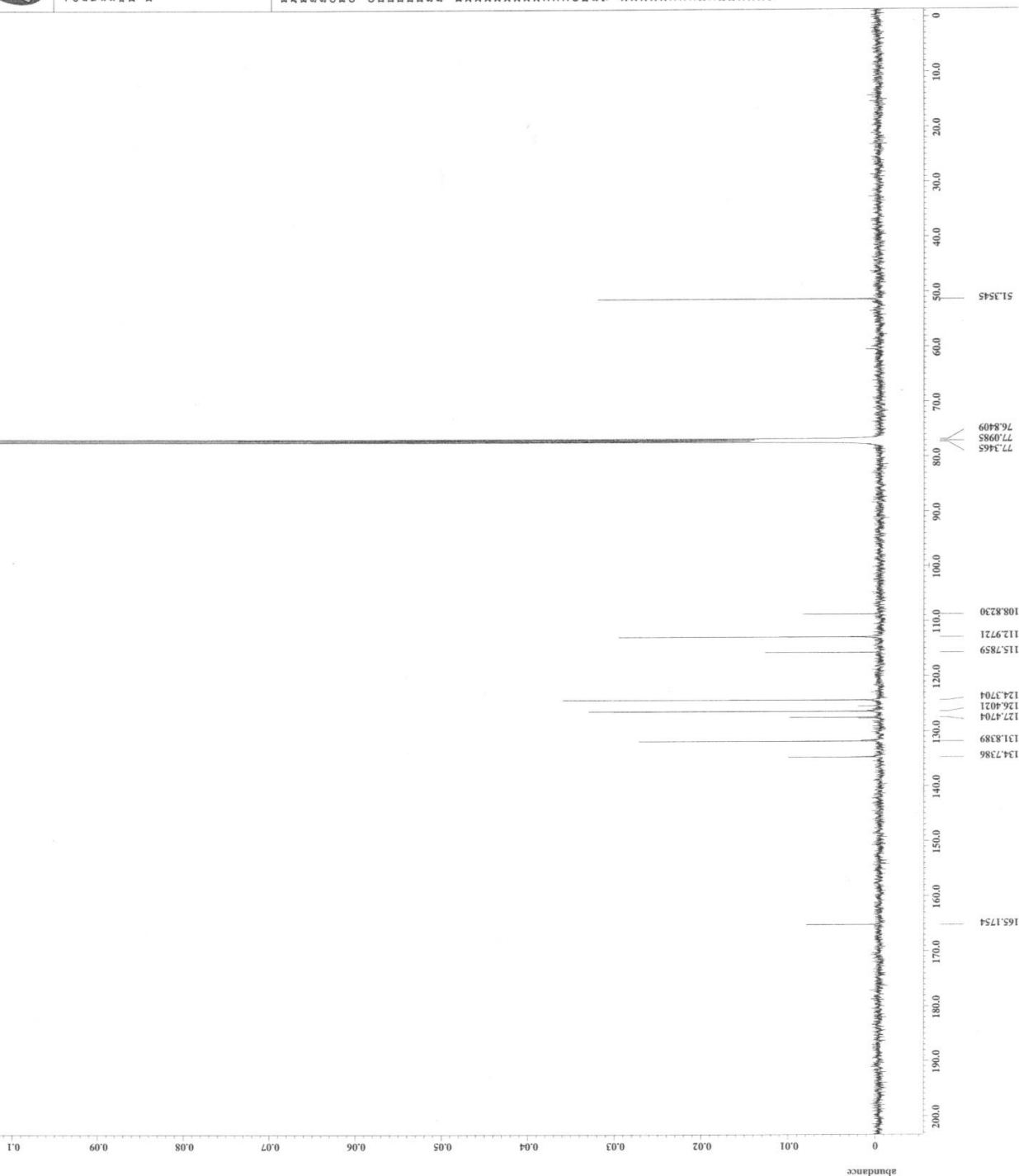
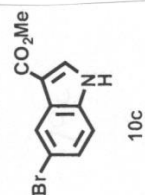
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Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dimensions = X [ppm]
Site = ECA500
Spectrometer = DELTAJ_NMR
Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_offset = 500.15991521 [MHz]
X_points = 5.0 [ppm]
X_resolution = 16384
X_sweep = 0.9727737 [Hz]
Irr_domain = 1H
Irr_offset = 9.38438438 [MHz]
Irr_freq = 500.15991521 [MHz]
Irr_points = 5.0 [ppm]
Trf_domain = 1H
Trf_freq = 500.15991521 [MHz]
Trf_offset = 9.38438438 [MHz]
Trf_points = 5.0 [ppm]
Mod_return = FALSE
Scans = 1
Total_scans = 8
X_90_width = 11.8 [us]
X_acq_time = 27.887904 [s]
X_delay = 25.44 [us]
X_atn = 3.4 [dB]
X_pulse = 5.9 [us]
X_mode = OFF
Trf_mode = OFF
Data_preset = FALSE
Initial_wait = 1 [s]
Acquire_wait = 1 [s]
Relaxation_delay = 5 [s]
Repetition_time = 6.74587904 [s]
Temp_get = 23 [C]



----- PROCESSING PARAMETERS -----
 dc balance : 0 : FALSE
 temp : 2.0 [Hz] : 0.0 [s]
 transpctd : 0 [N] : 80 [N] : 100 [N]
 resolution : 0.0 [Hz] : 0.0 [Hz]
 zft : 1 : TRUE : TRUE
 machine phase
 ppm

Derived from: 2016031601-3.jdf

Filename = 2016031601-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sampled = 128
 Solvent = CHLOROFORM-D
 Creation_time = 12-MAR-2016 01:24:134
 Revision_time = 17-MAR-2016 07:30:136
 Current_time = 17-MAR-2016 07:35:148
 Comment = single pulse decouple
 Data_format = 1D
 Data_title = 2D
 Dim_units = 13C
 Dimensions = [ppm]
 Size = KCAS00
 Spectrometer = DELTA2_NMR
 Field_strength = 11.742379 [T] (500 [MH])
 X_acq_duration = 0.83361792 [s]
 X_domain = 13C
 X_freq = 125.76529768 [MHz]
 X_offset = 0.0 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.1959034 [Hz]
 X_sweep = 0.3082761 [kHz]
 Ir_f_domain = 1H
 Ir_f_freq = 500.15941521 [MHz]
 Ir_offset = 0.0 [ppm]
 Ir_offset2 = 0.0 [ppm]
 Mod_return = 1
 Total_scans = 18320
 X_90_width = 11.3 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_pulse = 3.76666667 [us]
 Ir_atn_dec = 21.318 [dB]
 Ir_atn_rse = 21.318 [dB]
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Recv_time = 2002
 Recvr_gain = 56
 Relaxation_delay = 2 [s]
 Repetition_time = 2.03361792 [s]
 Temp_set = 24 [C]

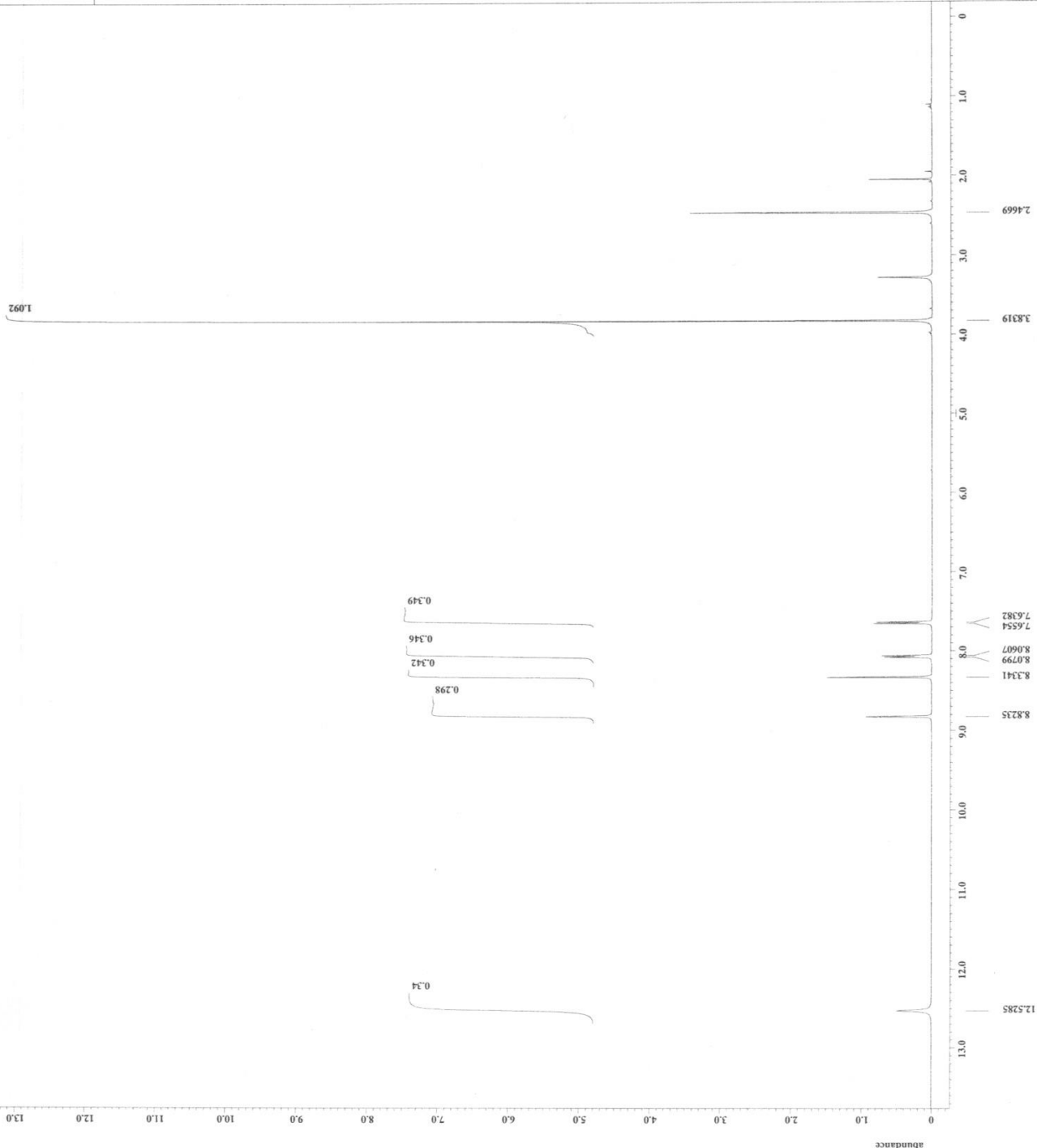
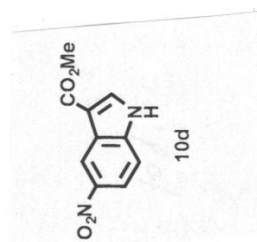


X : parts per Million : 13C

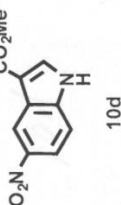
```

Filename = single_pulse-558.fdf
Author =
Experiment = single_pulse.ex2
Pulse_program = zgpg30
Solvent = DMSO-d6
Creation_time = 6-APR-2016 14:39:53
Revision_time = 6-APR-2016 15:57:55
Current_time = 6-APR-2016 15:57:07

Content =
  = single_pulse
  = 1D GPC/SEC
  = 1H
  = [ppm]
  = ECA 500
  = DELTA2_NMR
  = 11.52036431 [T] (500.1M)
  = 1.05644032 [s]
  = 495.11191398 [MHz]
  = 5 [ppm]
  = 13384
  = 1
  = 0.946575 [Hz]
  = 1H
  = 5068486 [Hz]
  = 495.11191398 [MHz]
  = 5 [ppm]
  = 13384
  = 495.11191398 [MHz]
  = 5 [ppm]
  = 7 [ALSE]
  = 1
  = 8
  = 12.6 [us]
  = 1.05644032 [s]
  = 45 [deg]
  = 6.5 [dB]
  = Off [us]
  = Off
  = Off
  = 1 [ALSE]
  = 44
  = 44
  = 5 [s]
  = 1.05644032 [s]
  = 24 [deg]
  = 24 [deg]
  
```

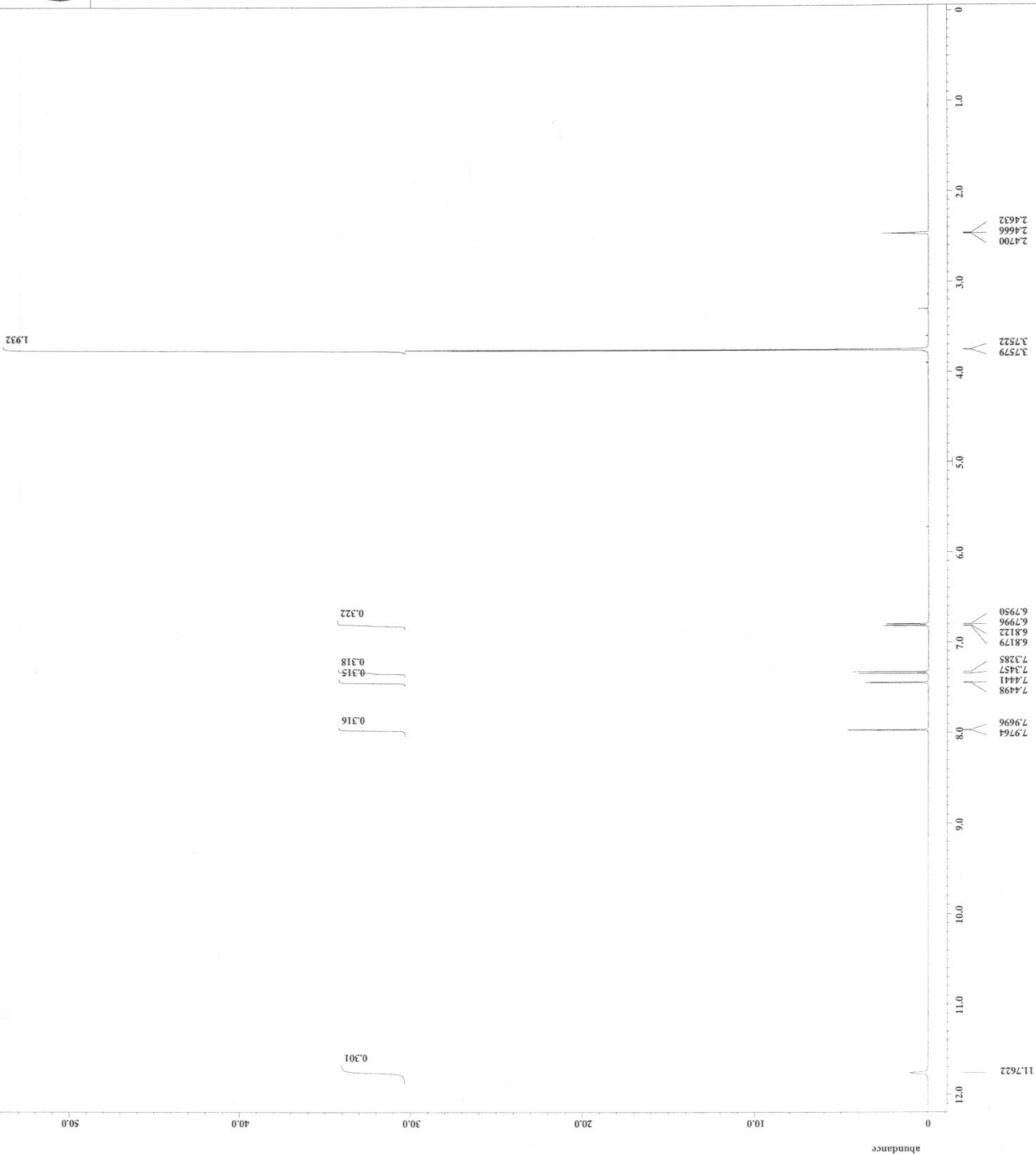
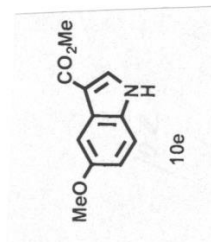


X : parts per Million : 1H



X : parts per Million : 13C

Filename = TAL60406-5.jdf
 Author =
 Date =
 Sample_id = 58686833
 Solvent = DMSO-d6
 Acquisition_time = 17:45:31
 Revision_time = 6-APR-2016 19:09:38
 Revision_time = 6-APR-2016 19:10:44
 Content = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dimensions = X [ppm]
 Site = ECA 500
 Spectrometer = DELTAJ_MMR
 Field_strength = 11.62926421(T) (500[M]
 X_acq_duration = 1.76422912[s]
 X_domain = 1H
 X_offset = 495.13191398[MHz]
 X_points = 5 [ppm]
 X_resolution = 16384
 X_sweep = 1
 X_center = 0.5668198[Hz]
 X_domain = 1H
 X_offset = 9.28677563[kHz]
 X_resolution = 495.13191398[MHz]
 X_sweep = 5 [ppm]
 X_domain = 1H
 Tr_freq = 495.13191398[MHz]
 Tr_offset = 5 [ppm]
 Mod_return = FALSE
 Scans = 1
 Total_scans = 8
 X_90_width = 12.6[us]
 X_acq_time = 1.76422912[s]
 X_center = 0.5668198[Hz]
 X_atn = 3.6[db]
 X_pulse = 6.3[us]
 Tr_mode = Off
 Tr_offset = Off
 Data_preset = FALSE
 Initial_wait = 1[s]
 Recv_gain_delay = 6[s]
 Repetition_time = 6.76422912[s]
 Temp_get = 23.7[dc]

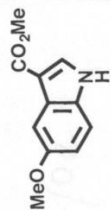


X : parts per Million : 1H

```

=====
Filename      = TA160406-4.jdf
Author        =
Experiment    =
Sample_id     = S468434
Solvent       = DMSO-d6
Acquisition_time = 7-APR-2016 06:53:48
Current_time  = 7-APR-2016 08:10:51
Content       =
=====
1D pulse decouple
=====
Data format   = 1D COMPLEX
Dir_size      = 26214
Dir_title     =
Dimensions    = 13C
Spectrometer  = ECA 500
Site          = DELTA2_MMR
Field strength = 11.62526421[T] (500[M]
X_acq_duration = 0.8386608[s]
X_domain      = 13C
X_offset      = 50.0059 [MHz]
X_points      = 1001
X_prescans    = 32768
X_resolution  = 4.192028 [Hz]
X_sweep       = 39.0625 [Hz]
X_domain      = 1H
X_freq        = 495.1191398 [MHz]
X_offset      = 0.0000 [MHz]
X_phase       = FALSE
Mod_return    = 1
Scans         = 16501
Total_scans   = 16501
X_90_width    = 10.5 [us]
X_acq_time    = 0.8386608[s]
X_resolution  = 9.8 [Hz]
X_atn         = 9.8 [dB]
X_pulse       = 3.5 [us]
X_atn_dec     = 20.86835 [dB]
X_atn_dec     = 20.86835 [dB]
X_atn_dec     = TRUE
Decoupling    = TRUE
Initial_wait  = 2 [s]
Noe_time      = 2 [s]
Recvr_gain    = 60
Relaxation_delay = 1.0 [s]
Relaxation_time = 2.8386608[s]
Temp_Set      = 24.5 [C]
=====

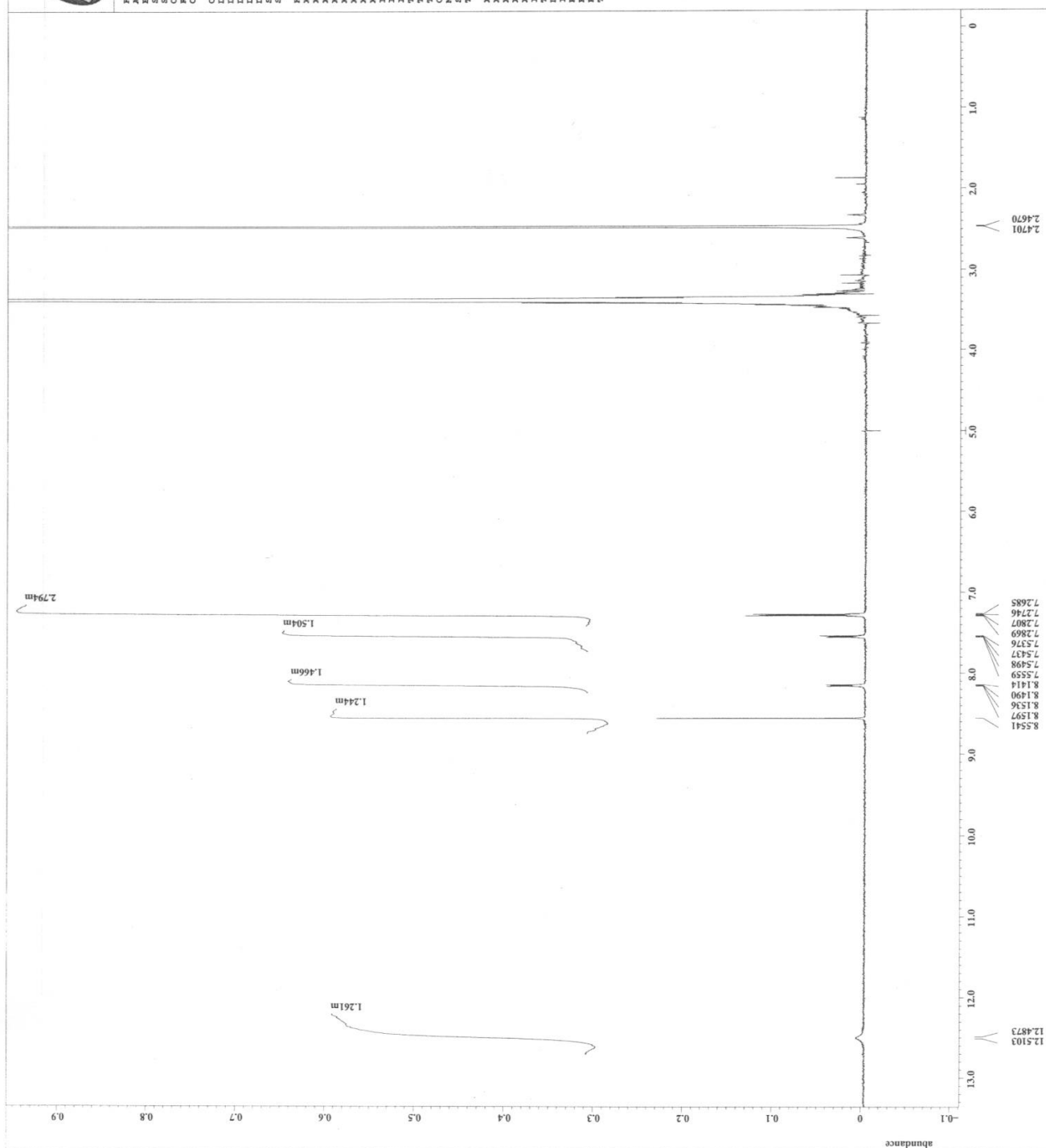
```



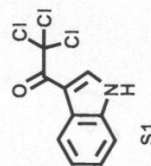
10e



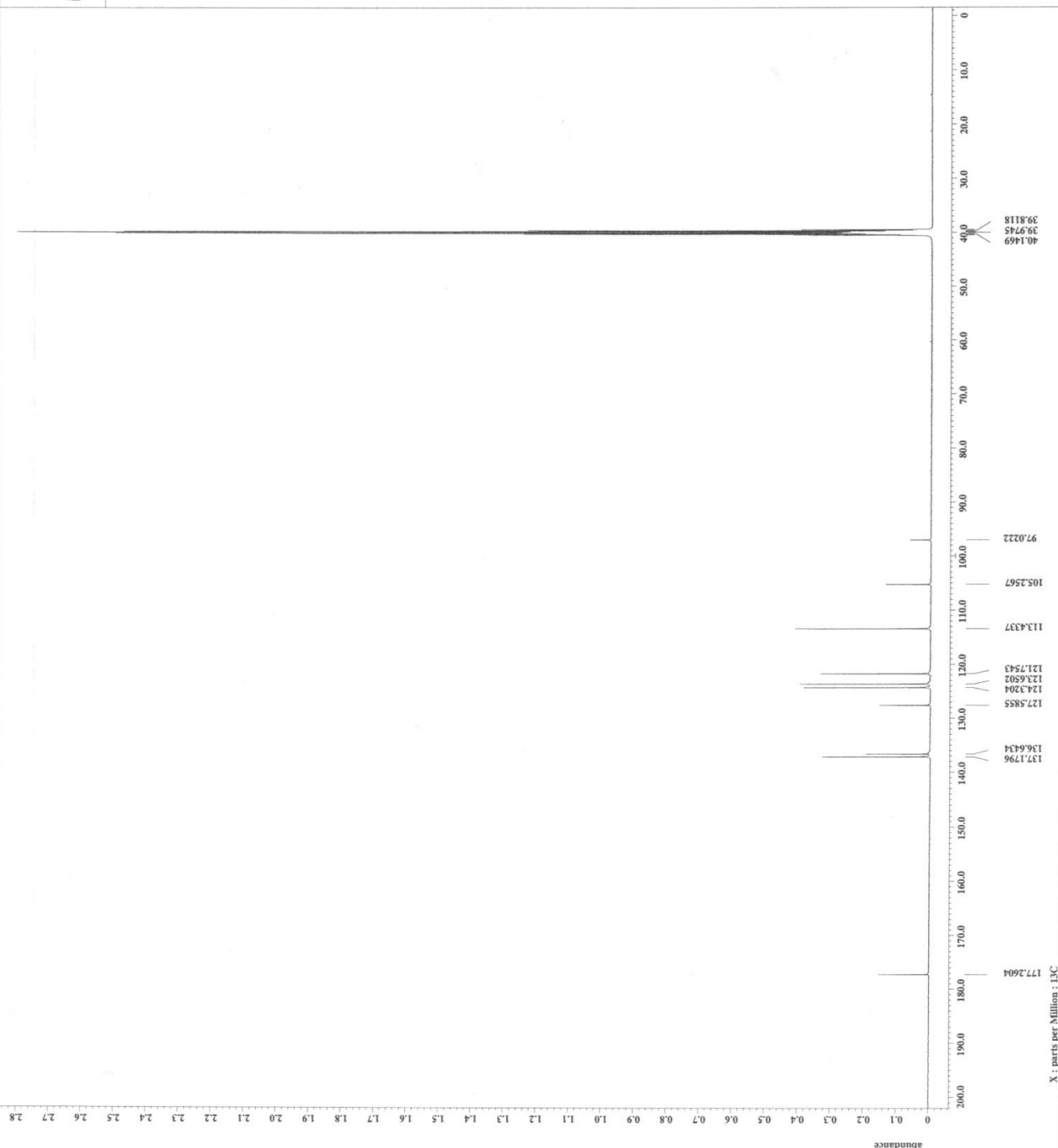
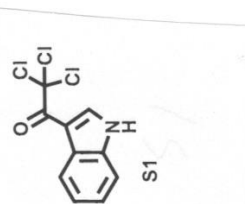
X: parts per Million : 13C



X : parts per Million : 1H



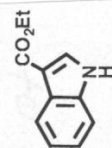
Filename = TAL60824-10.jdf
 Author =
 Experiment =
 Solvent =
 Solvent_id =
 Creation_time =
 Acquisition_time =
 Current_time =
 Content =
 Content_comment =
 Dim_title =
 Dim_units =
 Dimensions =
 Site =
 Spectrometer =
 Field_strength =
 X_acq_duration =
 X_domain =
 X_freq =
 X_offset =
 X_points =
 X_prescans =
 X_resolution =
 X_sweep =
 Ir_freq =
 Ir_domain =
 Ir_offset =
 Ir_noise =
 Mod_return =
 Scans =
 Total_scans =
 X_90_width =
 X_acq_time =
 X_delay =
 X_atn =
 X_pulse =
 Ir_noise_dec =
 Ir_atn_dec =
 Ir_noise =
 Decoupling =
 Nuttall_wait =
 Noe_time =
 Recv_gain =
 Recv_delay =
 Repetition_time =
 Temp_get =



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```
----- PROCESSING PARAMETERS -----  
dnc_balance : 0 : FALSE  
freq_exp : 0.2[Hz] : 0.0[s]  
fraprazold3 : 0[%] : 80[%] : 100[%]  
microfill : 1  
nfft : 1 : TRUE : TRUE  
machinephase  
ppm  
Derived from: TA160407-7.jdf
```

Derived from: TA160407-7.jde

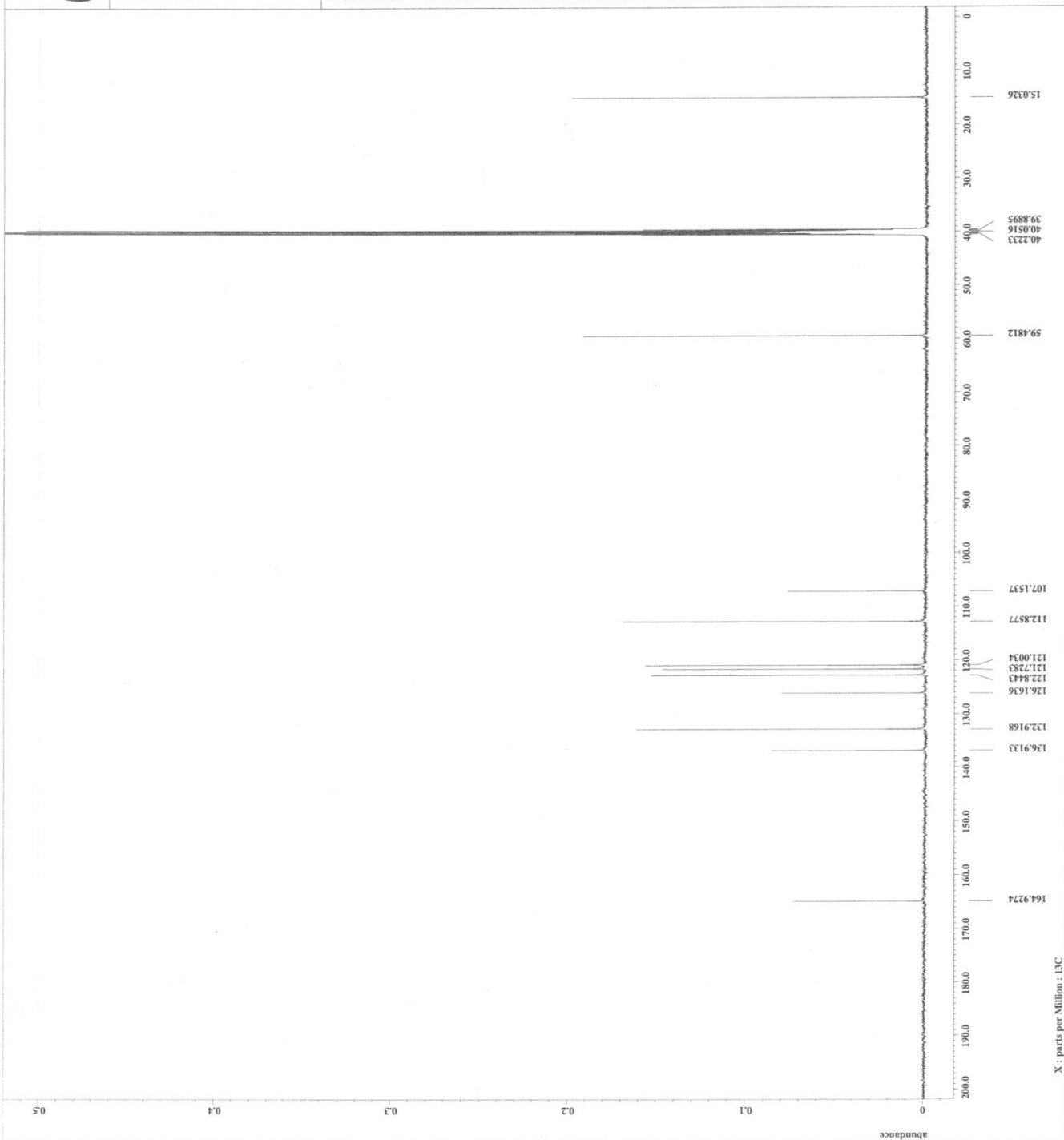
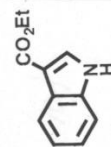
[illegible]

1 of 1

X : parts per Million : 1H

----- PROCESSING PARAMETERS -----
 dc_balance : 0.000000
 trap_sol_d3 : 0.000000
 zero_fill : 1
 mach_phase : TRUE
 ppm
 Derived from: TAI60407-10.jdf

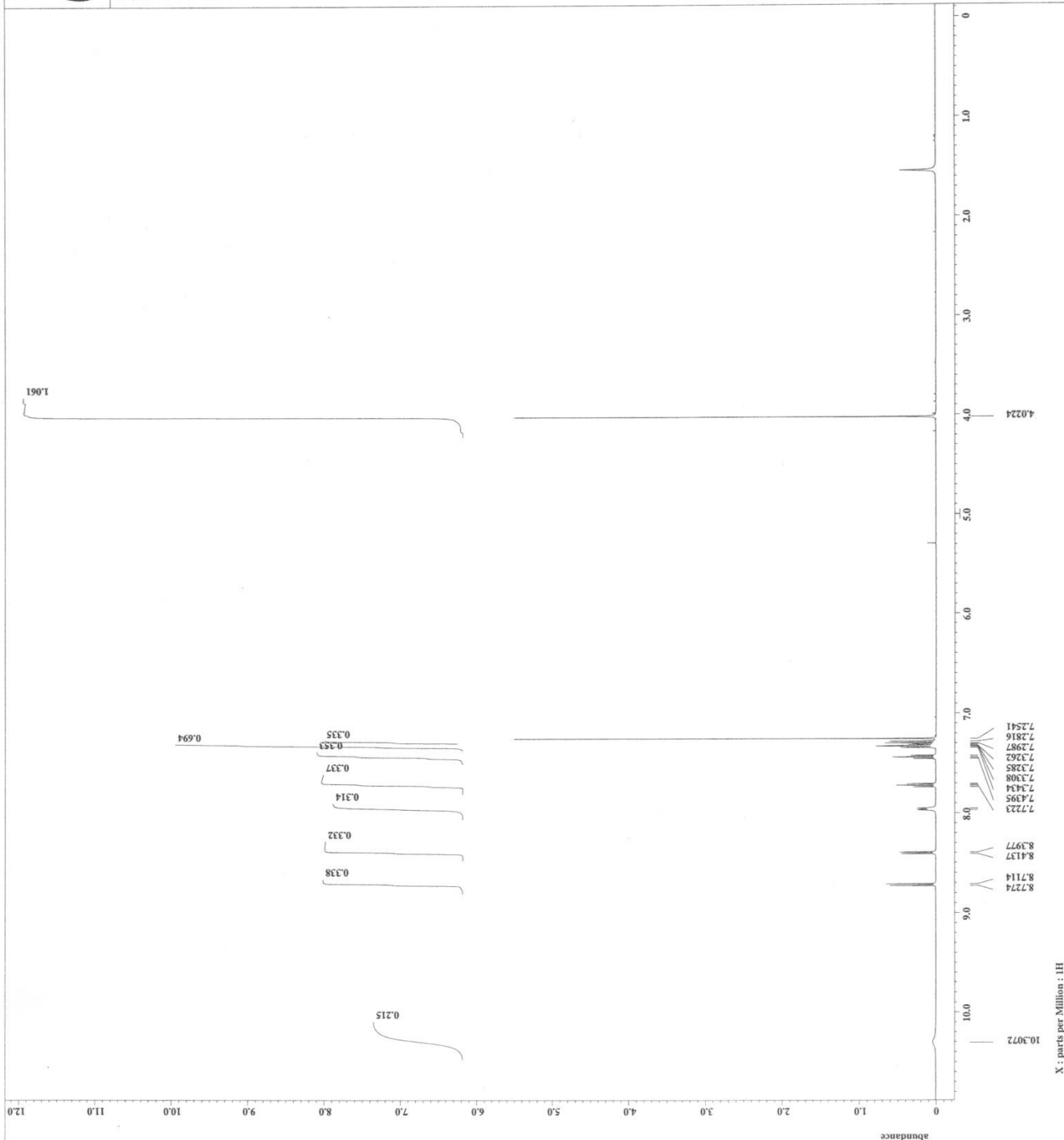
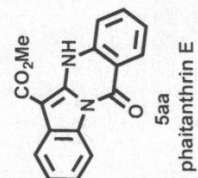
File name = TAI60407-11.jdf
 Acquisition = single_pulse_dec
 Sample_id = S8521535
 Date_ = 2016-04-07 11:25:02
 Revision_time = 7-APR-2016 17:13:13
 Current_time = 7-APR-2016 17:13:18
 Comment = single pulse decouple
 Data_format = ID COMPLEX
 Dim_size = 28214
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = DEPTA_NMR
 Field_strength = 11.7473573 [T] (500 [MH]
 X_acq_duration = 0.83361792 [s]
 X_freq = 125.76539768 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_resolution = 1.19959034 [Hz]
 X_sweep = 39.3081761 [kHz]
 X_domain = 100.15991521 [MHz]
 X_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Total_scans = 3838
 X_90_width = 11.3 [us]
 X_90_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 5.5 [dB]
 X_pulse = 2.766667 [us]
 X_pulse_dec = 21.318 [dB]
 Irr_atn_noe = 21.318 [dB]
 Irr_noise = WALTZ
 Decoupling = 110
 Initial_pit = TRUE
 Noe_time = 2 [s]
 Repetition_delay = 2 [s]
 Repetition_time = 2.83361792 [s]
 Temp_set = 23.3 [C]



```

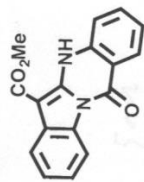
=====
File      T150427-10.jdx
Name      T150427-10.jdx
Author    T150427-10.jdx
Experiment single_pulse.exe
Sample_id 08349300
Date      27-APR-2016 08:24:39
Creation_time
Revision_time
Current_time
Content
Data_format 1D COMPLEX
Dir_name 1107
Dir_units 1H
Dimensions 1
Spectrometer JNM-500
P1 1.00
DELTA2_NMR
=====
Field_strength 11.6224421[T] (500[M
X_domain 1H
X_freq 495.1313398[MHz]
X_offset 5[ppm]
X_resolution 0.566198[Hz]
X_sweep 0.566198[Hz]
X_acq_time 1.7642291[s]
X_angle 45[deg]
X_atn 1.5[dB]
X_mode Off[us]
X_trf_mode Off
Data_preset FALSE
Relaxation_delay 2[s]
Repetition_time 2.7642291[s]
Temp_set 24.7[degC]
=====

```

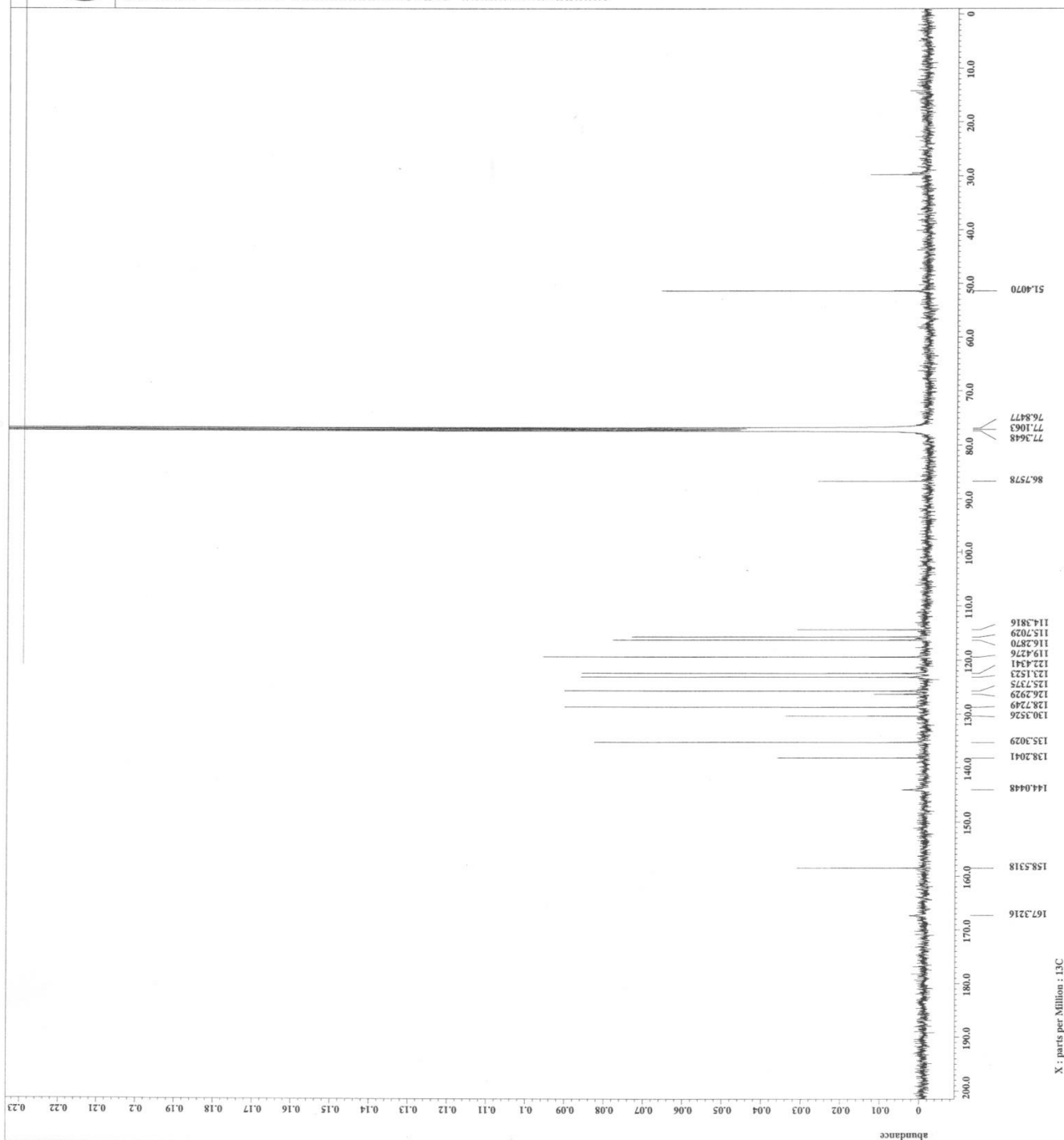


```

=====
File Name      : 5a11104_copy-4.jdf
Experiment     : single_pulse_dec
Sample ID      : 88587718
Date_ Acq      : 5-NOV-2014 07:16:19
Creation Time   : 5-NOV-2014 07:10:20
Revision Time   : 5-NOV-2014 07:13:39
Current Time    :
Content         : single pulse decouple
Data Format     : 1D COMPLEX
Dir Size       : 24214
Dir Units      : [s]
Dir Units       : [ppm]
Dimensions     : X
Site           : ECA 500
Spectrometer   : JEOLJNMNR
Field Strength : 11.62926421[T] (500[M]
X_Acq Duration : 1.8388608[s]
X_Freq         : 124.5010059[MHz]
X_Offset       : 100[ppm]
X_Points       : 4
X_Resolution   : 1.192029[Hz]
X_Sweep        : 35.0625[MHz]
X_Acquire      : 495.13191398[MHz]
Irr_Freq       : 5[ppm]
Irr_Offset     : FALSE
Clipped        : TRUE
Mod Return     : 1
Scans          : 19077
Total Scans    : 19077
X_90_Width     : 10.4[us]
X_Acq Time     : 0.8388608[s]
X_Angle        : 30[deg]
X_Pulse        : 3.4666667[us]
Irr_Atn_Dec    : 20.86935[db]
Irr_Atn_Pwr    : 20.86935[db]
Decoupling     : TRUE
Initial Wait   : 1[s]
Noe Time       : 2[us]
Recvr Gain     : 60
Relaxation_Delay : 2[s]
Repetition Time : 2.8388608[s]
Temp_Set       : 24[deg]
=====
  
```



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X : parts per Million : 13C

0.342

```

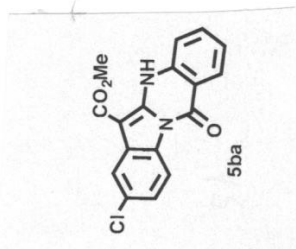
= 20150404-5C1-4_jdf
Author = daica
Experiment = single_pulse_ox2
Sample_id = DMSO-16
Solvent = DMSO-16
Creation_time = 4-APR-2016 11:55:24
Revision_time = 4-APR-2016 13:14:51
Current_time = 4-APR-2016 13:14:54

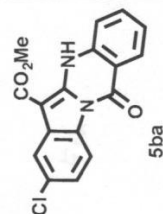
Content = single_pulse
Data_format = 1D COMPLEX
Data_size = 1H 307
Dm_title = [ppm]
Dm_units = [ppm]
Dimensions = 500
Spectrum = DELTA2_NMR

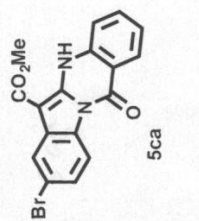
Field_strength = 1H 430.6421(2) (500[M]
Spectrum = 1H 7.64429212(a)
X_domain = 1H
X_freq = 495.1191398 [MHz]
X_points = 10384
X_resolution = 0.56618 [Hz]
X_rsd = 1H 887.563 [Hz]
Ir_domain = 495.1191398 [MHz]
Ir_offset = 5 [ppm]
Ir1_freq = 495.1191398 [MHz]
Ir1_offset = 5 [ppm]
Clipped = FALSE
Scans = 8
Total_scans = 8

X90_width = 12.5 [us]
X90_time = 1.76428212(a)
X_angle = 45 [deg]
X_pulse = 6.3 [us]
X_pulse = 6.3 [us]
Ir_mode = Off
Ir_offset = Off
Initial_wait = 1(s)
Recirc_gain = 48
Relaxation_delay = 5.5 [s]
Relaxation_time = 22.916212(a)
Temp_set = 22.916212(a)
Temp_gpt = 22.916212(a)

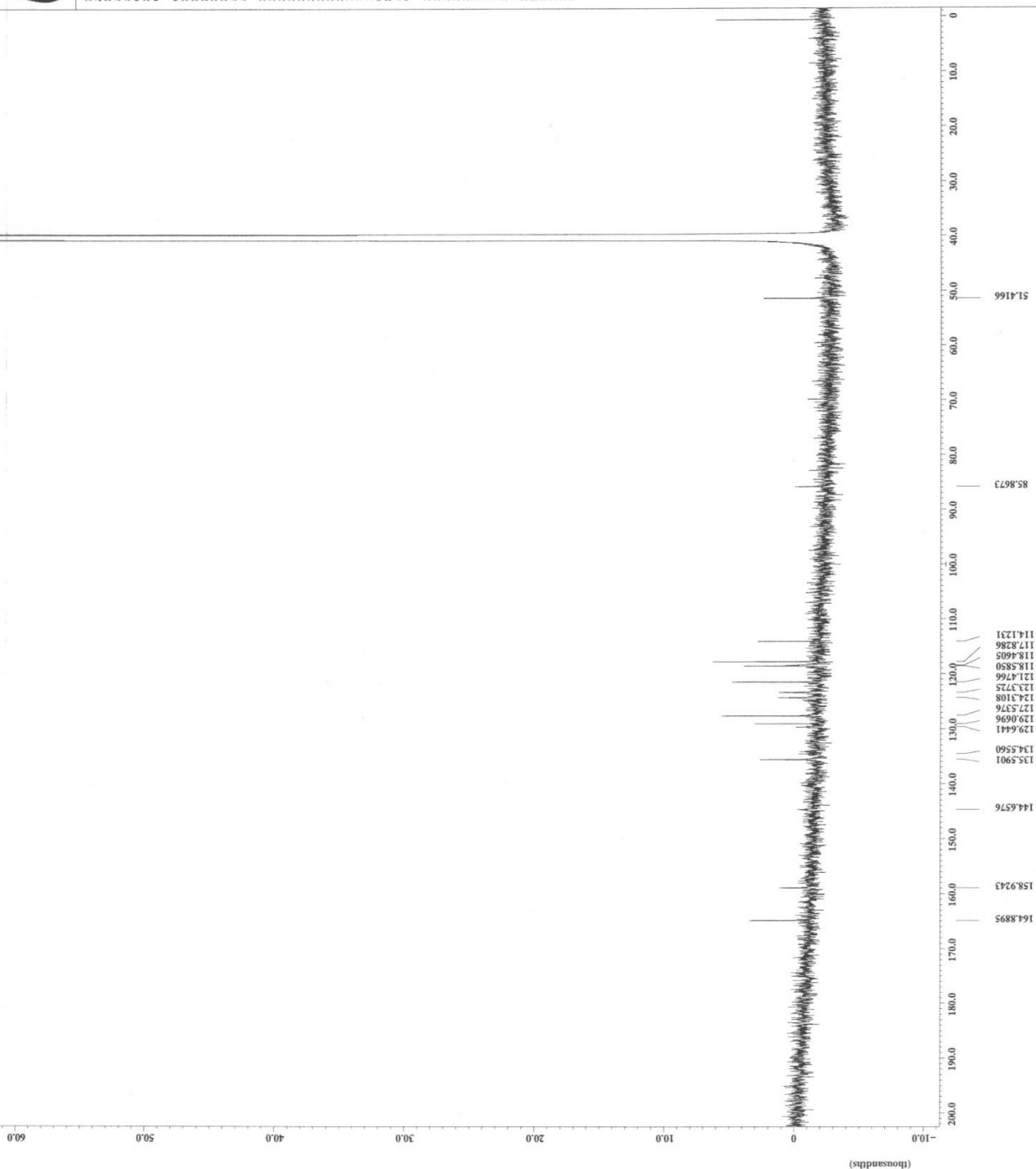
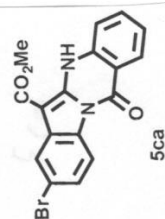
```





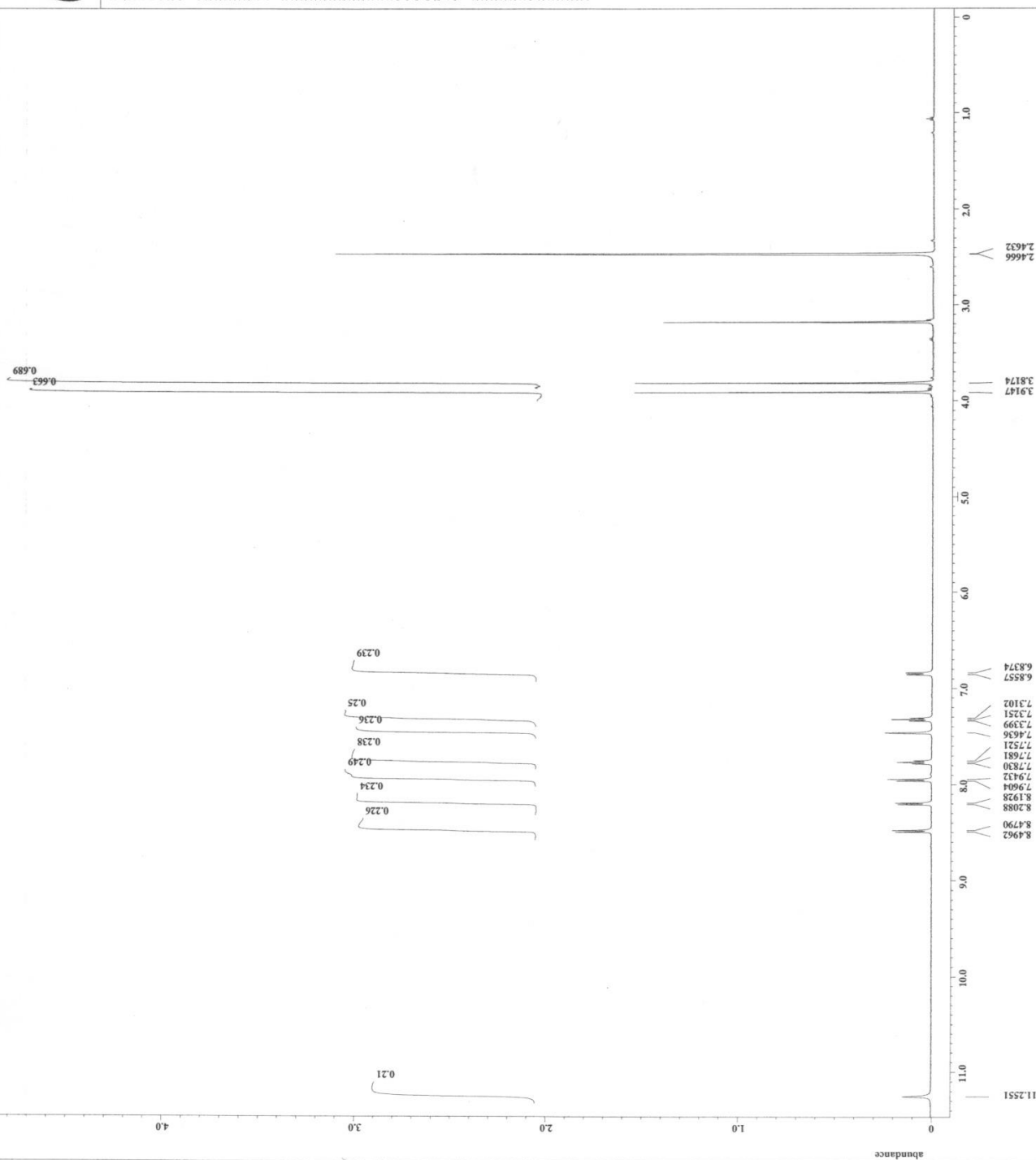
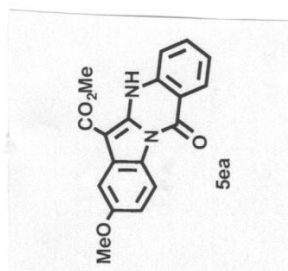


Filename	= Data0415-4_jdf
Author	= single_pulse_dec
Experiment	= DMSO-D6
Solvent	= DMSO-D6
Creation_time	= 10-APR-2016 09:47:40
Creation_time	= 10-APR-2016 11:11:39
Current_time	= 10-APR-2016 11:13:31
Content	= single pulse decouple
Data format	= 1D COMPLEX
F1 file name	= 13C
F2 file name	= 13C
F3 file name	= [ppm]
D1a units	= KHz
Dimensions	= KXZ 500
Spectrometer	= DRZ42A_NMR
Probe strength	= 13.52906321 [%] (500 MHz)
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.9010095[MHz]
X_resolution	= 32749
X_points	= 4
X_prescan	= 1.1202927[Hz]
Y_acq_duration	= 13.7625[sec]
Y_domain	= 495.13191398[MHz]
Y_freq	= 5(ppm)
Y_offset	= 1
Modeof_return	= OFFSET
Total_scans	= 78622
X_30_width	= 10.5[us]
X_acq_time	= 0.8388608[s]
Z_acq_time	= 13.7625[sec]
Z_angle	= 9.81[deg]
Z_pulse	= 3.5[us]
Ir_rfreq	= 20.68935[dd]
Ir_rdecoupling	= 20.68935[dd]
Ir_noise	= MZR2
Decoupling	= TRUE
Initial_wait	= 1[s]
Noise	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Relaxation_time	= 0.8388608[s]
Post_gst	= 50.1[sec]

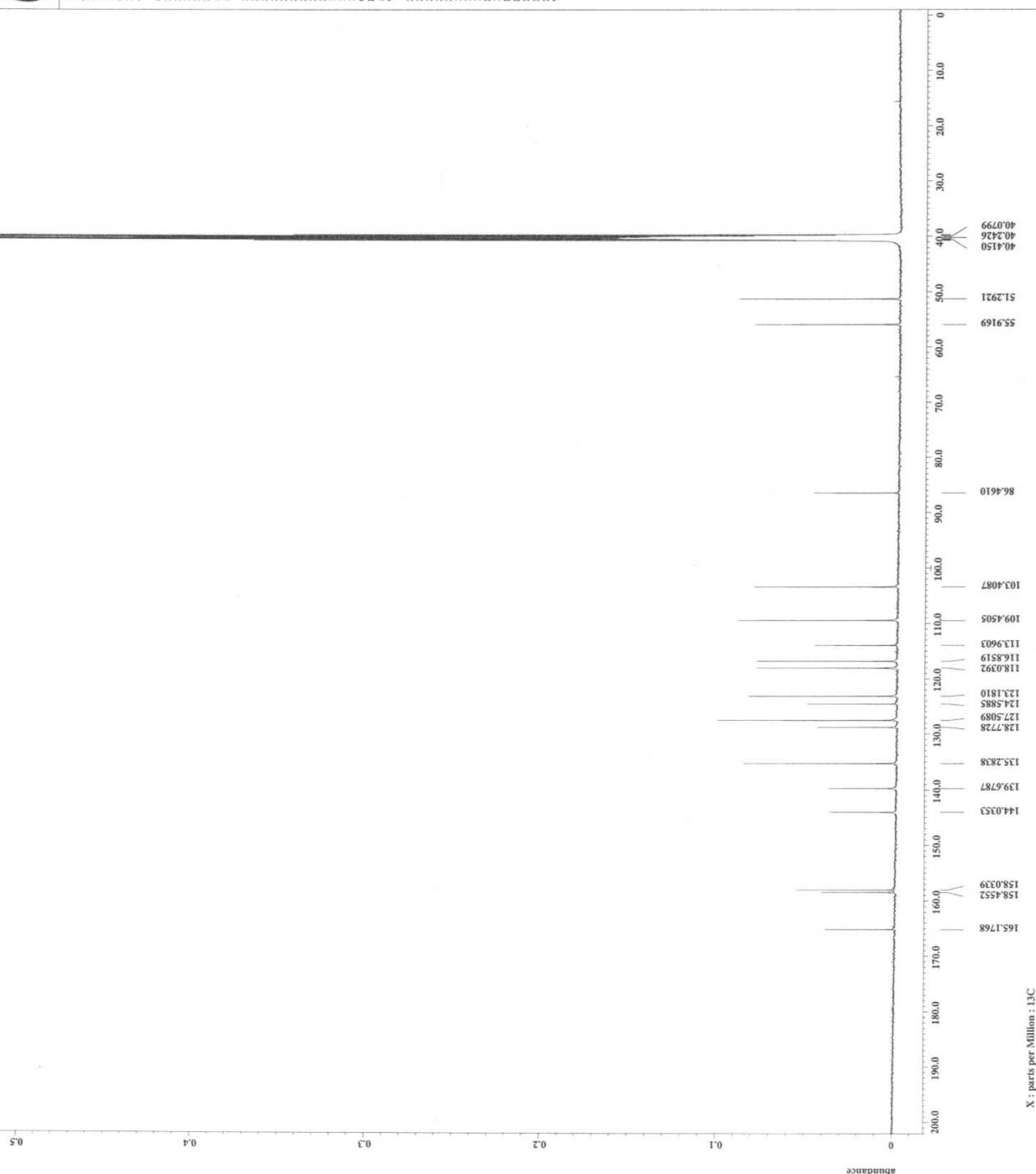
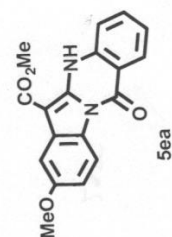


X : parts per Million : 13C

```
= IY020160408-Step-4_3.spc  
= data  
= single_pulse.asx  
Experiment =  
ID         = DMSO-D6  
Solvent    =  
Creation_time   = 8-APR-2016 14:09:29  
Revision_time  = 8-APR-2016 15:28:20  
Current_Time   = 8-APR-2016 15:29:04  
  
Content      = single_pulse  
             = 1D COMPLEX  
             = 17  
             = 1H  
           [ppm]  
Dimensions   = XZ, Y0  
F2            = KZA 500  
Spectrum     = DELTA2_NMR  
  
Field_strength  = 11.629563(17) [500 MHz]  
X_acq_duration  = 1.76422912(s)  
X_domain        = 1H  
X_freq          = 495.13191398 [MHz]  
X_points        = 10394  
X_resolution    = 1  
X_scales        = 0.5688198 [Hz]  
              = 2.8677503 [kHz]  
Y_domain        = 1H  
Y_freq          = 495.13191398 [MHz]  
Y_points        = 5 [ppm]  
Y_resolution    = 5 [ppm]  
Y_scales        = 5 [ppm]  
Z_domain        = 7 kHz  
Z_freq          = 7 kHz  
Z_points        = 8  
Z_resolution    = 8  
Z_scales        = 8  
Total_scans     = 12.6 (usl)  
X_90_width      = 1.76422912(s)  
X_acq_time      = 1.76422912(s)  
X_angle         = 45[deg]  
X_phase         = 6.3 [deg]  
X_pulse         = 6.3 [usl]  
Prg_name        = OFZ  
Tr_mode         = OFF  
Tr_offset       = 0  
Initial_wait    = 46  
Recvr_gain      = 46  
Relaxation_delay = 5.4422912(s)  
Repeat_time     = 5.4422912(s)  
Scan_percent    = 50.1 [dc]
```



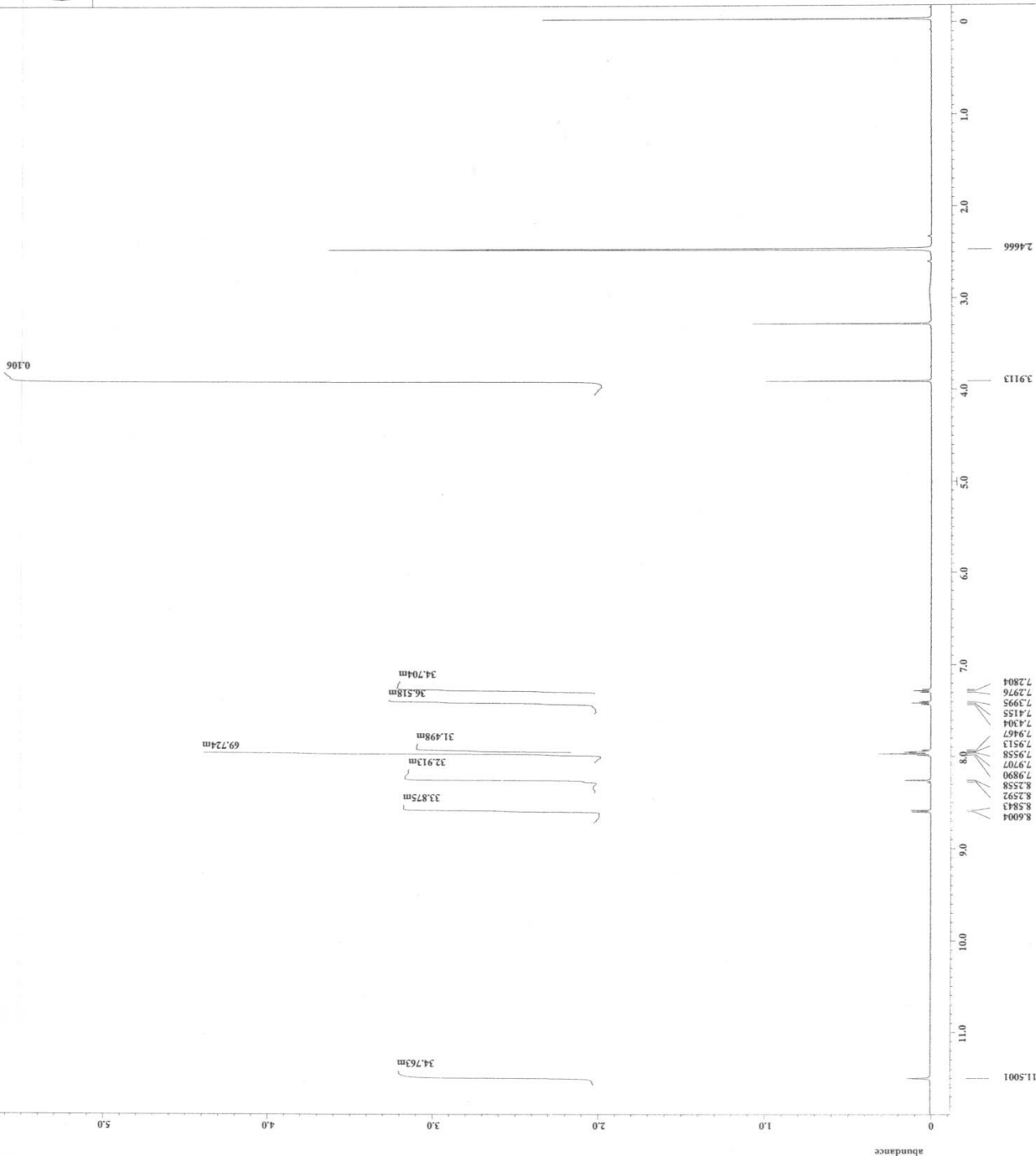
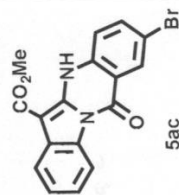
X : parts per Million : 1H



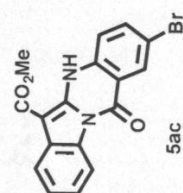
```

=====
Filename      = TAI60315-3.jdr
Experiment     = single_pulse.ex2
Sample_id      = S852728
Solvent        = DMSO-d6
Acq_date       = 15-MAR-2016 14:11:47
Revision_time  = 15-MAR-2016 15:26:12
Current_time   = 15-MAR-2016 15:26:18
Content        = single_pulse
Data_format    = 1D COMPLEX
Dim_size       = 13107
Dim_unit       = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = DELTAJ_500
Field_strength = 11.6226421[T] (500[M]
X_acq_duration = 1.76422212[s]
X_domain       = 1.76422212[s]
X_freq         = 495.13191398[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_resolution   = 0.5668198[Hz]
X_sweep        = 9.2867563[Hz]
Xf_domain      = 495.13191398[MHz]
Xf_offset      = 5[ppm]
Tr_domain      = 1H
Tr_freq        = 495.13191398[MHz]
Tr_offset      = 5[ppm]
Tr_resolution   = 0.5668198[Hz]
Mod_return     = 1
Scans          = 8
Total_scans    = 8
X_90_width     = 12.6[us]
X_acq_time     = 1.76422212[s]
X_gate         = 45[us]
X_atn          = 3.6[db]
X_pulse        = 6.3[us]
Tr_mode        = Off
Tr_offset      = Off
Dante_preset   = FALSE
Initial_wait   = 1[s]
Relaxation_delay = 8[s]
Repetition_time = 6.76422912[s]
Temp_get       = 23.5[degC]
=====

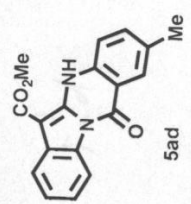
```

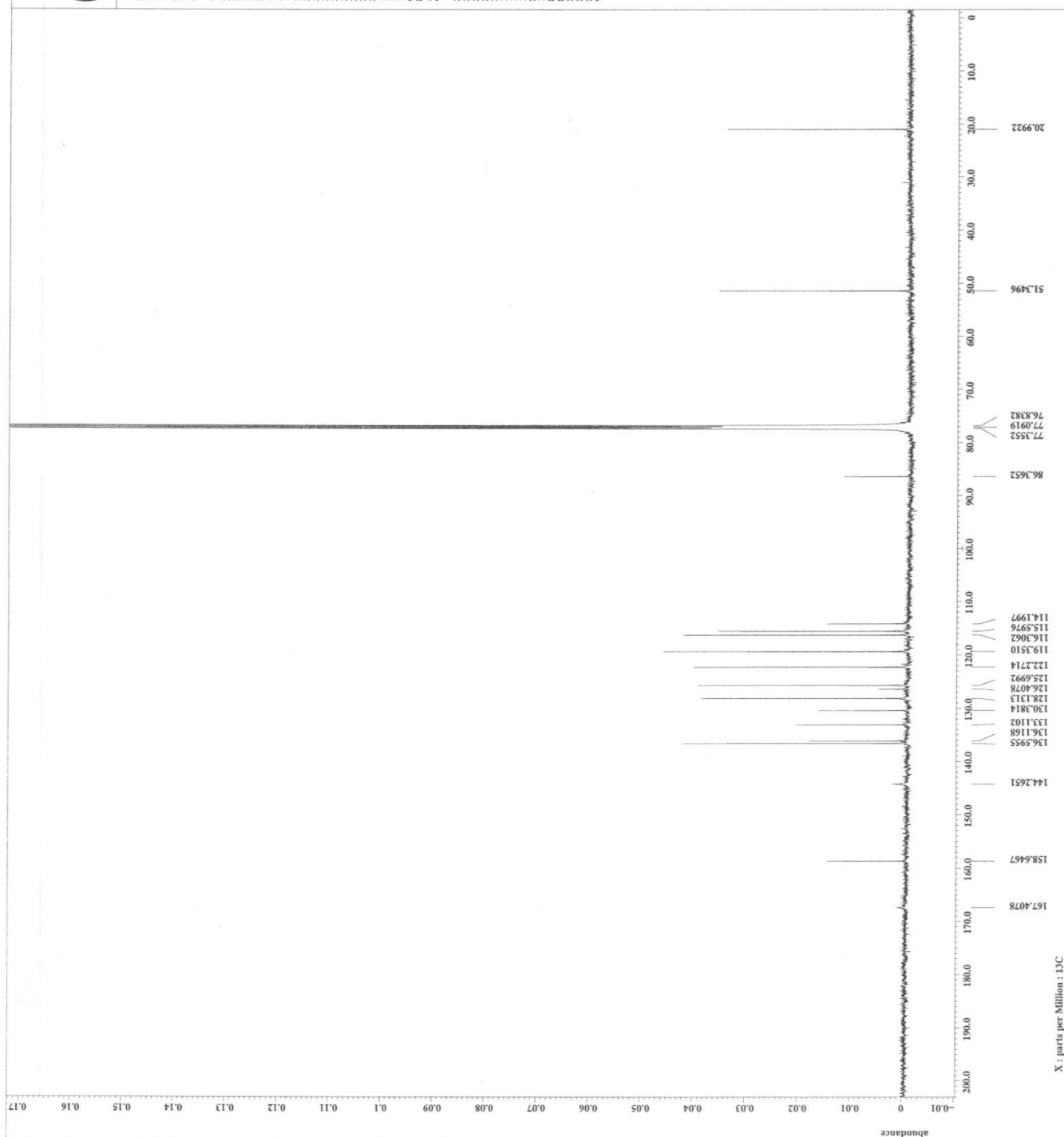
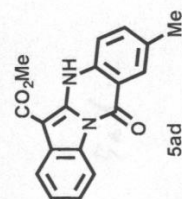


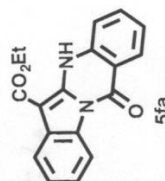
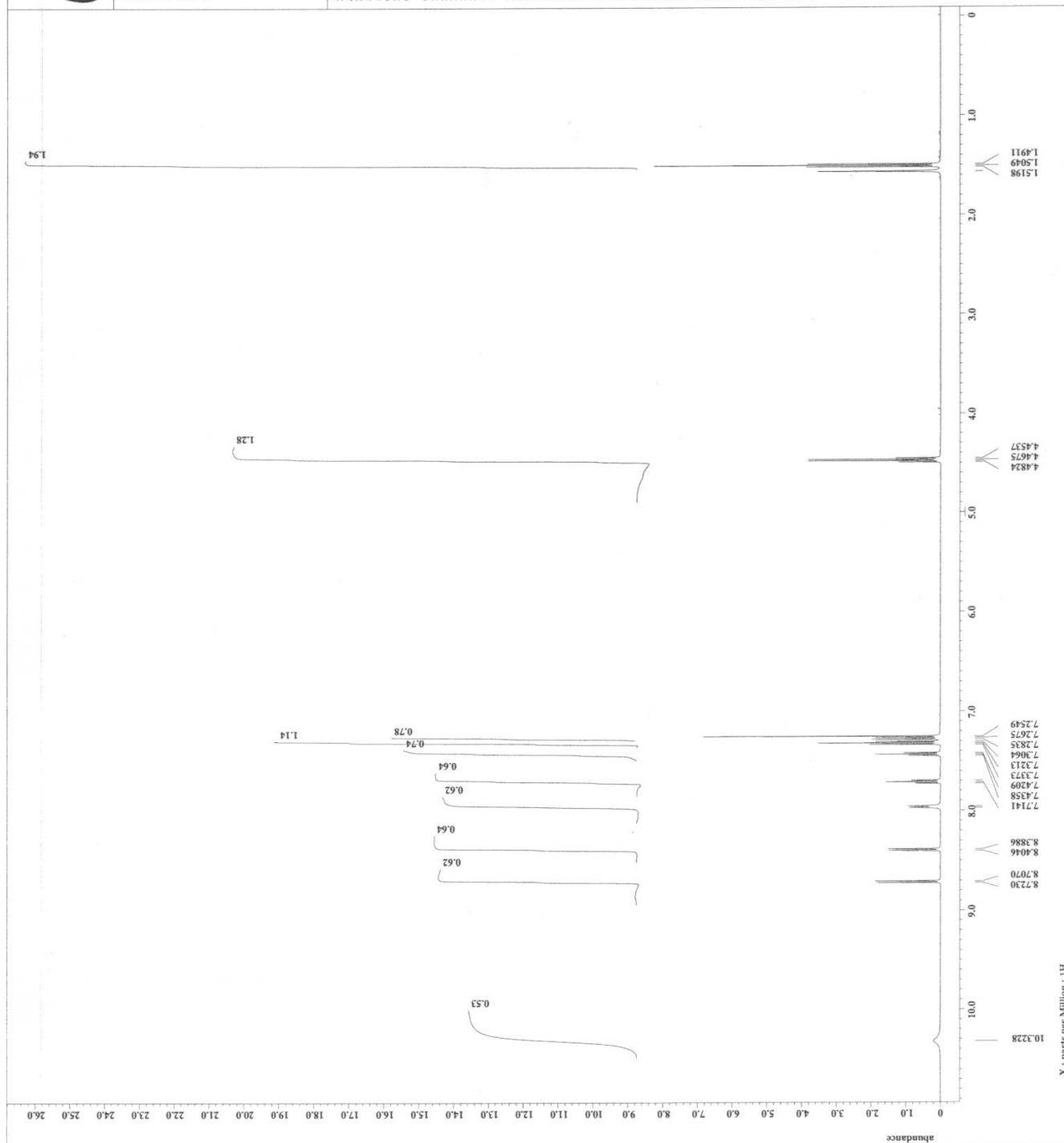
X : parts per Million : 1H



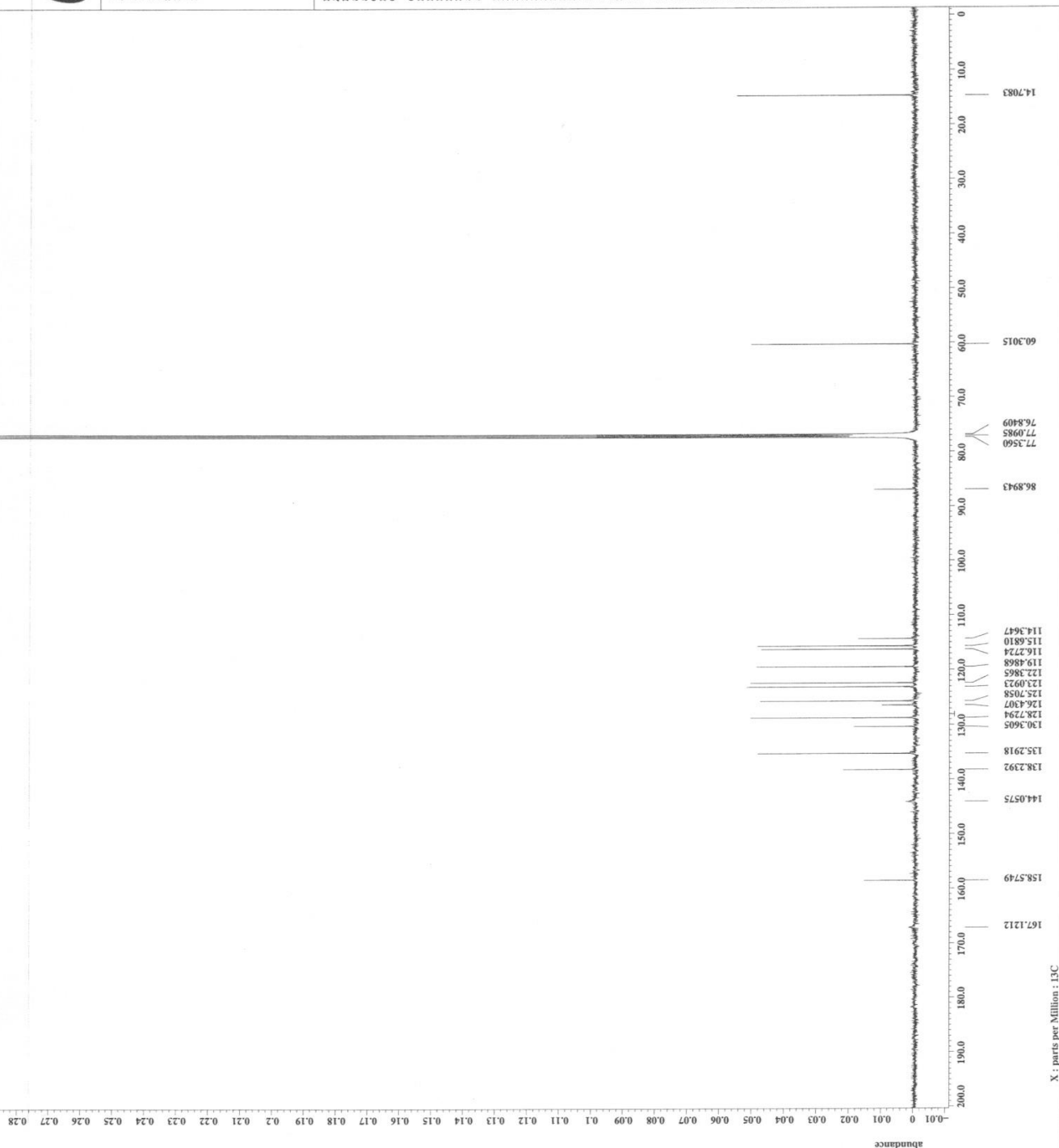
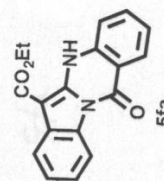
5ac



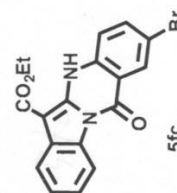
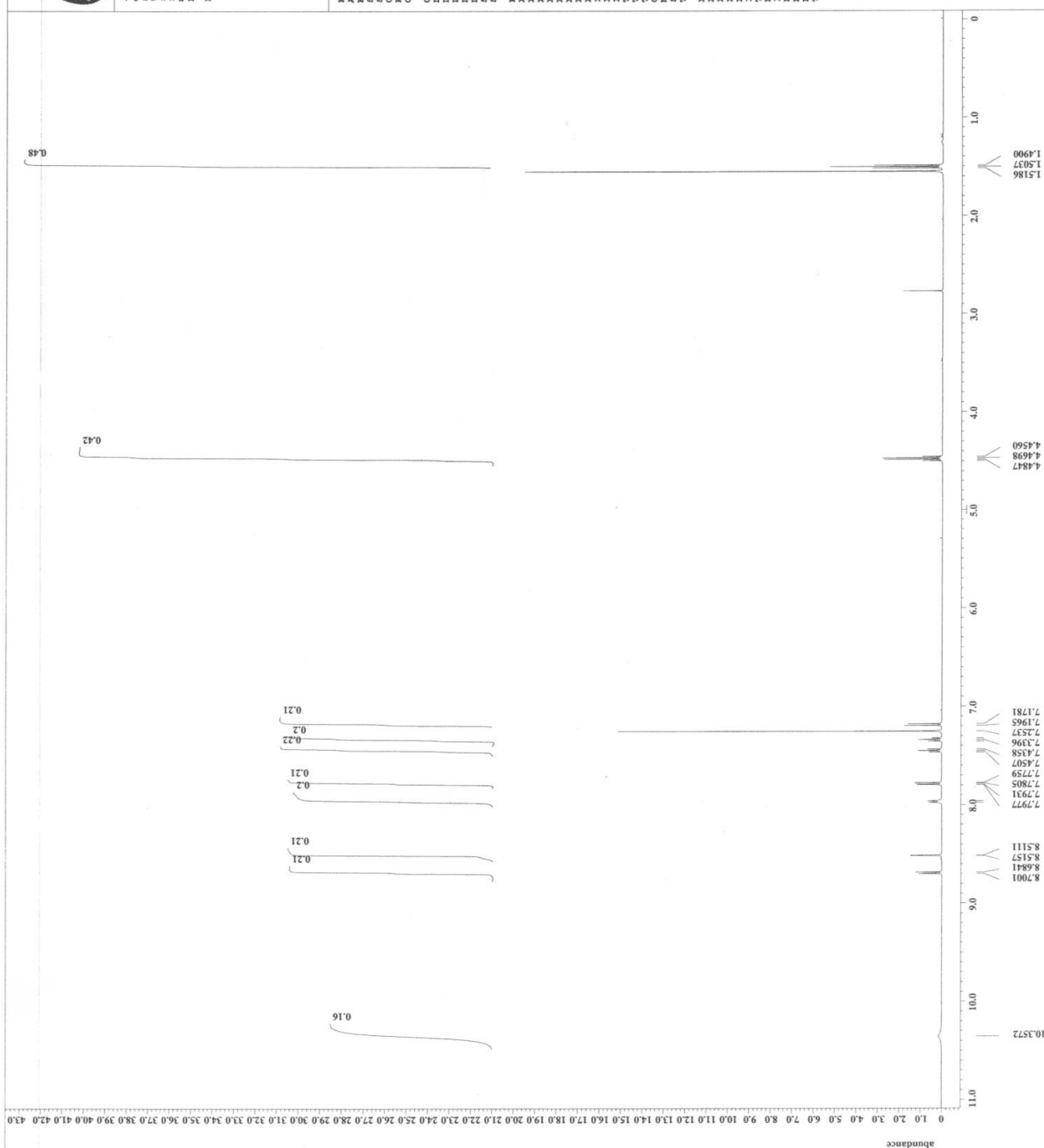


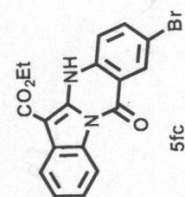


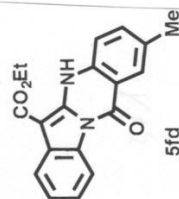
Derived from: TA160330-10.jdf

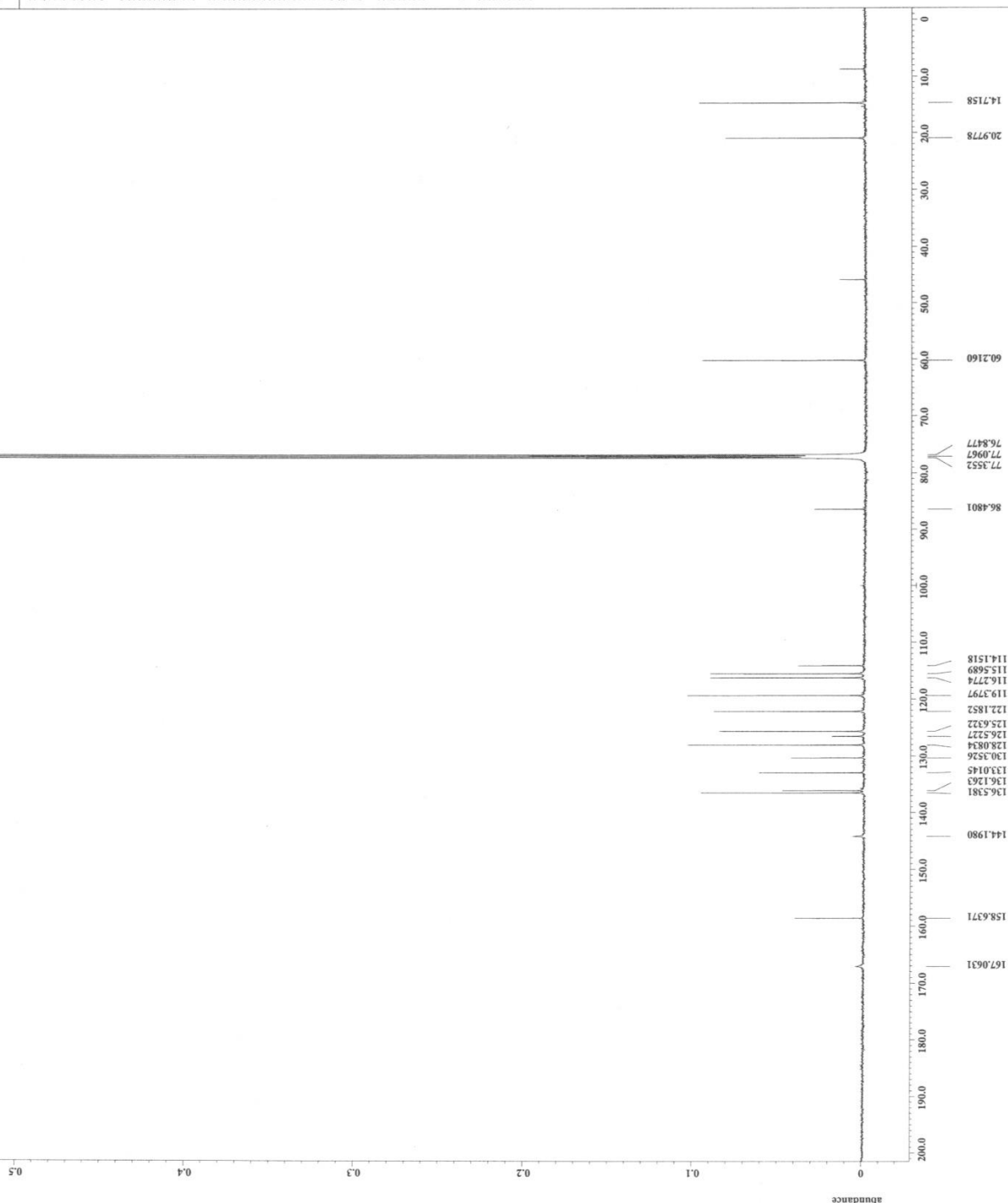
[illegible]


Derived from: TA160331-1.jdf











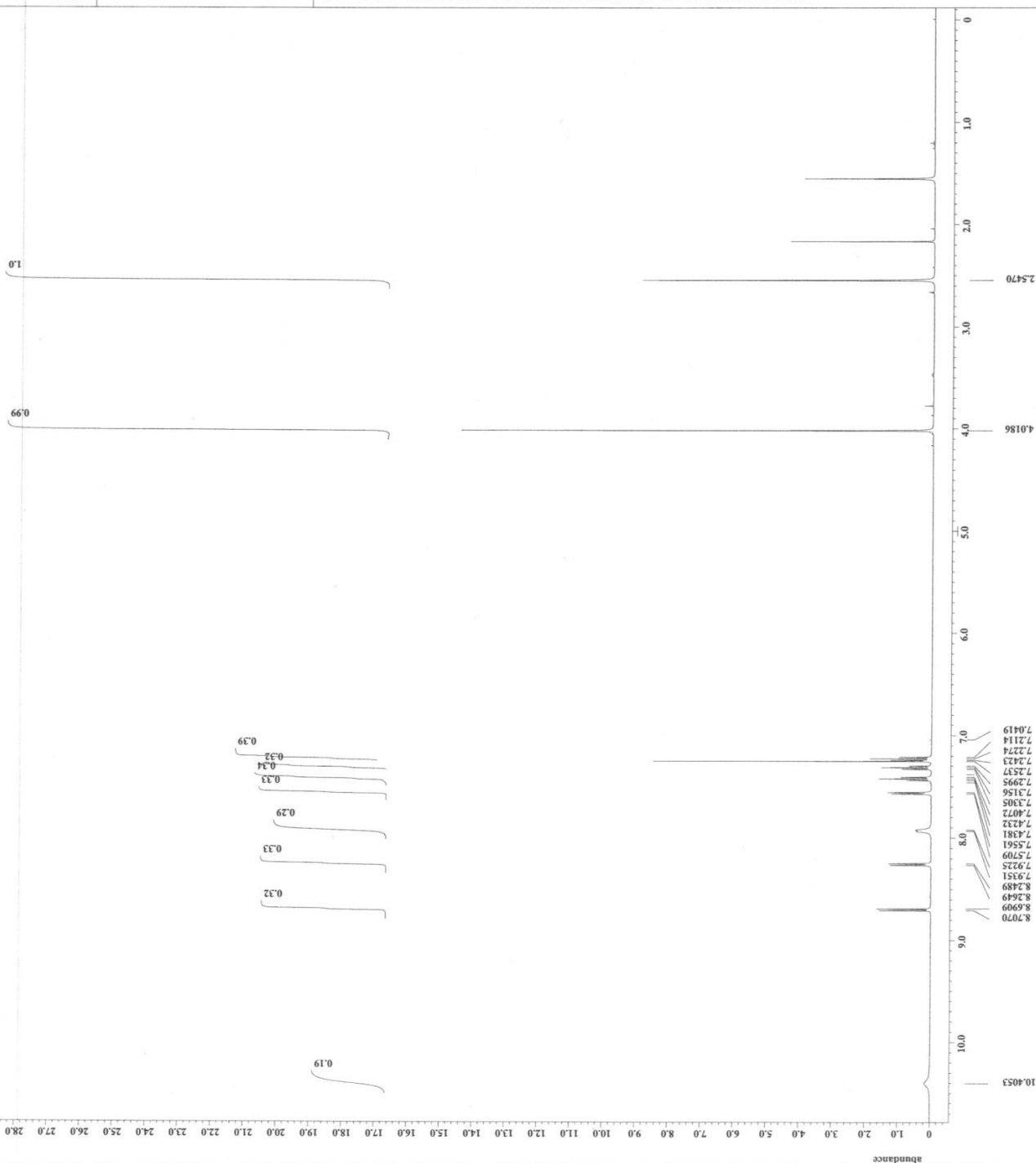
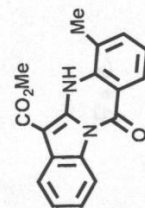
```

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

```

Derived from: TA160317-5.jdf

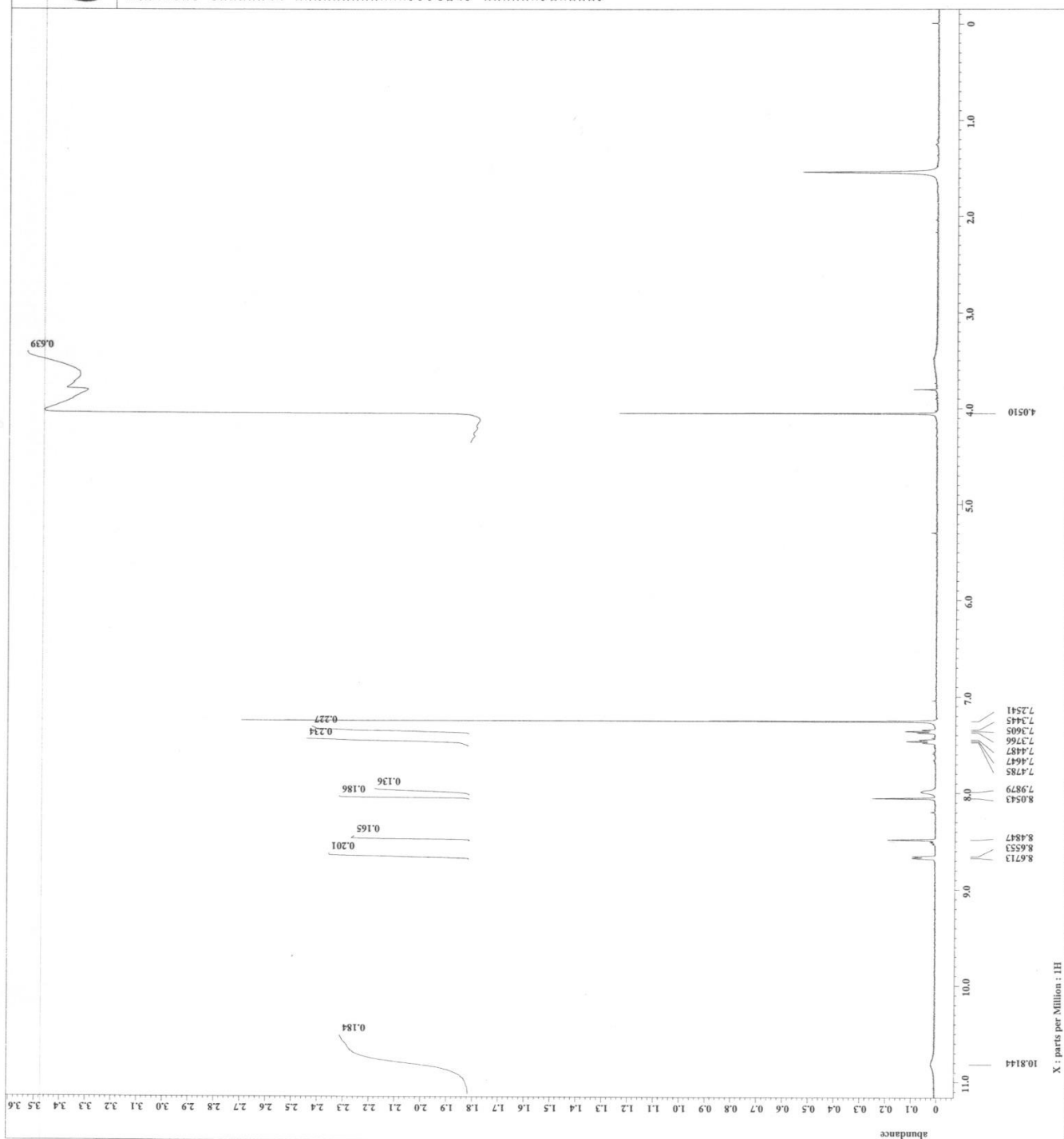
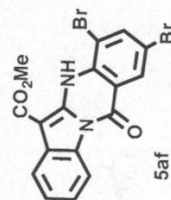
Filename	"data0317-7_jd6"	
Author	"dela"	
Experiment	"single_pulse_ex2"	
ExperimentId	"17-03-2016-01"	
Solvent	"CHLOROFORM-D"	
Creation_time	"13-MAR-2016 07:45:27"	
Revision_time	"17-MAR-2016 13:53:05"	
Revision_time	"17-MAR-2016 13:54:26"	
Comment	"single_pulse"	
Unit	"Hz"	
Data format	"1D COMPLEX"	
File name	"17-03-2016-01"	
File path	"13"	
File units	"[ppm]"	
Dimensions	"X Y Z"	
Dimensions	"X Y Z"	
Spectrometer	"XEN500"	
Procesor	"DELTA2_NMR"	
1D strength	"1.74759794(s)"	(500 [MHz]
2D strength	"1.74587904(s)"	
3D strength	"18"	
4D strength	"18"	
5D strength	"500.15994521 [MHz]"	
6D strength	"500.15994521 [MHz]"	
7D strength	"16384"	
8D strength	"1"	
9D strength	"0.57277737 [Hz]"	
10D strength	"3.34358438 [MHz]"	
11D strength	"18"	
12D strength	"5.0 [ppm]"	
13D strength	"5.0 [ppm]"	
14D strength	"500.15994521 [MHz]"	
15D strength	"5.0 [ppm]"	
16D strength	"FALDZ"	
17D strength	"FALDZ"	
18D strength	"8"	
19D strength	"8"	
20D strength	"11.8 [us]"	
21D strength	"1.74587904(s)"	
22D strength	"45 [deg]"	
23D strength	"5 [deg]"	
24D strength	"5 [deg]"	
25D strength	"Off"	
26D strength	"Off"	
27D strength	"11.8 [us]"	
28D strength	"11.8 [us]"	
29D strength	"58"	
30D strength	"1.74587904(s)"	
31D strength	"22.8 [deg]"	
32D strength	"22.8 [deg]"	
33D strength	"22.8 [deg]"	
34D strength	"22.8 [deg]"	
35D strength	"22.8 [deg]"	
36D strength	"22.8 [deg]"	
37D strength	"22.8 [deg]"	
38D strength	"22.8 [deg]"	
39D strength	"22.8 [deg]"	
40D strength	"22.8 [deg]"	
41D strength	"22.8 [deg]"	
42D strength	"22.8 [deg]"	
43D strength	"22.8 [deg]"	
44D strength	"22.8 [deg]"	
45D strength	"22.8 [deg]"	
46D strength	"22.8 [deg]"	
47D strength	"22.8 [deg]"	
48D strength	"22.8 [deg]"	
49D strength	"22.8 [deg]"	
50D strength	"22.8 [deg]"	
51D strength	"22.8 [deg]"	
52D strength	"22.8 [deg]"	
53D strength	"22.8 [deg]"	
54D strength	"22.8 [deg]"	
55D strength	"22.8 [deg]"	
56D strength	"22.8 [deg]"	
57D strength	"22.8 [deg]"	
58D strength	"22.8 [deg]"	
59D strength	"22.8 [deg]"	
60D strength	"22.8 [deg]"	
61D strength	"22.8 [deg]"	
62D strength	"22.8 [deg]"	
63D strength	"22.8 [deg]"	
64D strength	"22.8 [deg]"	
65D strength	"22.8 [deg]"	
66D strength	"22.8 [deg]"	
67D strength	"22.8 [deg]"	
68D strength	"22.8 [deg]"	
69D strength	"22.8 [deg]"	
70D strength	"22.8 [deg]"	
71D strength	"22.8 [deg]"	
72D strength	"22.8 [deg]"	
73D strength	"22.8 [deg]"	
74D strength	"22.8 [deg]"	
75D strength	"22.8 [deg]"	
76D strength	"22.8 [deg]"	
77D strength	"22.8 [deg]"	
78D strength	"22.8 [deg]"	
79D strength	"22.8 [deg]"	
80D strength	"22.8 [deg]"	
81D strength	"22.8 [deg]"	
82D strength	"22.8 [deg]"	
83D strength	"22.8 [deg]"	
84D strength	"22.8 [deg]"	
85D strength	"22.8 [deg]"	
86D strength	"22.8 [deg]"	
87D strength	"22.8 [deg]"	
88D strength	"22.8 [deg]"	
89D strength	"22.8 [deg]"	
90D strength	"22.8 [deg]"	
91D strength	"22.8 [deg]"	
92D strength	"22.8 [deg]"	
93D strength	"22.8 [deg]"	
94D strength	"22.8 [deg]"	
95D strength	"22.8 [deg]"	
96D strength	"22.8 [deg]"	
97D strength	"22.8 [deg]"	
98D strength	"22.8 [deg]"	
99D strength	"22.8 [deg]"	
100D strength	"22.8 [deg]"	



K : parts per Million : 1H

5ae

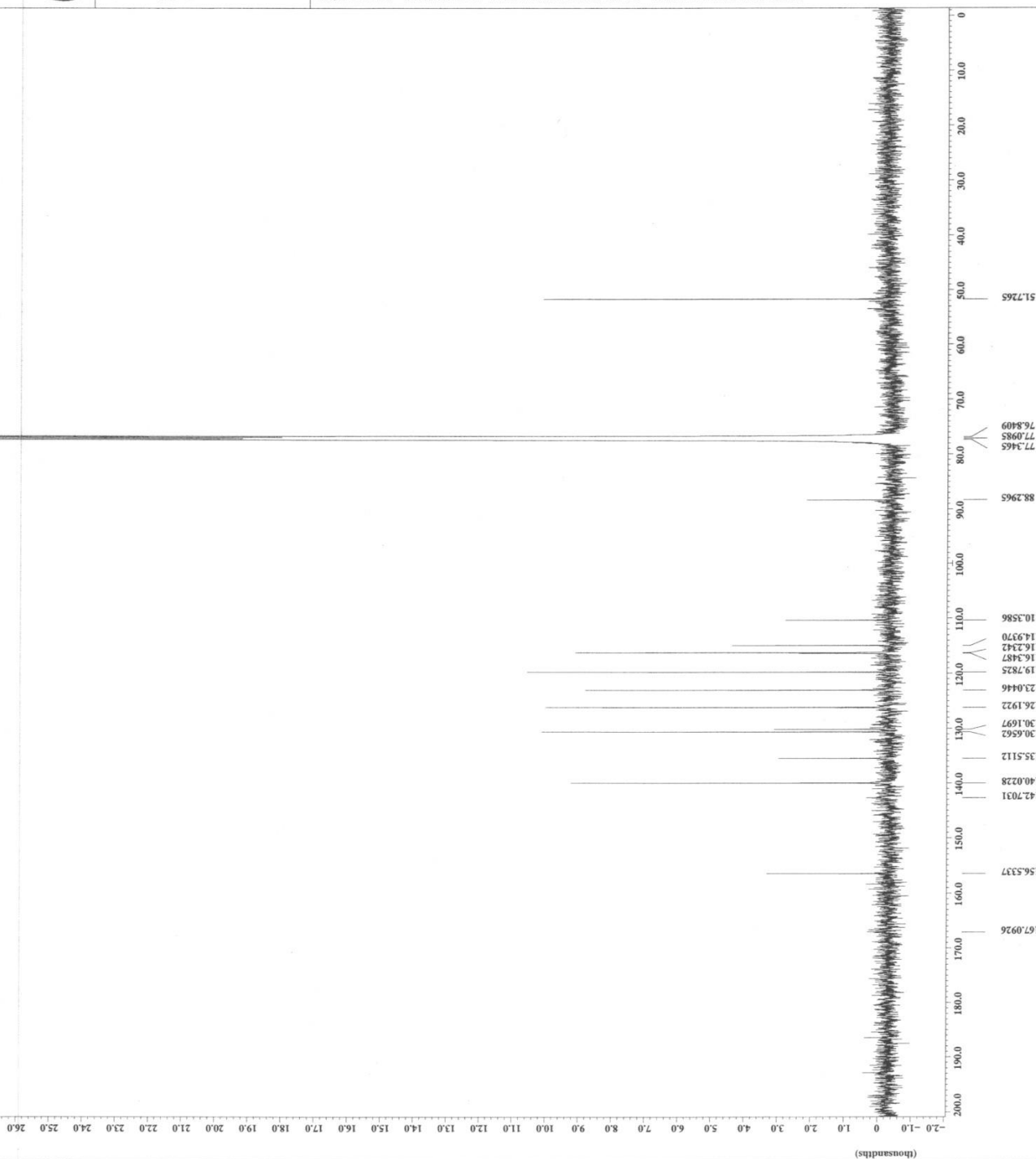
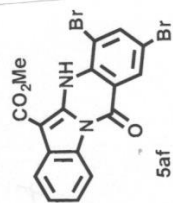
Filename = TA100318-3-jdf
 Experiment = single_pulse.exe
 Sample_id = 58303912
 Solvent = CHLOROFORM-D
 Acq_date_time = 18-MAR-2016 07:16:27
 Revision_time = 18-MAR-2016 08:32:50
 Current_time = 18-MAR-2016 08:32:55
 Content = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dimensions = X
 Site = ECA 500
 Spectrometer = DELTAJ_NMR
 Field_strength = 11.62926421[T] (500[M
 X_acq_duration = 1.76422912[s]
 X_domain = 1H
 X_offset = 495.13191398[MHz]
 X_points = 512ppm
 X_resolution = 16384
 X_sweep = 0.56681981[Hz]
 Irr_domain = 1H
 Irr_offset = 9.248677563[MHz]
 Tri_domain = 1H
 Tri_freq = 495.13191398[MHz]
 Tri_offset = 16ppm
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8
 X_90_width = 12.6[us]
 X_acq_time = 1.76422912[s]
 X_offset = 3.6[us]
 X_pulse = 6.3[us]
 Irr_mode = Off
 Irr_offset = 0.2[us]
 Data_presat = FALSE
 Initial_wait = 1[s]
 Recv_gain = 48
 Repetition_delay = 1.0[s]
 Repetition_time = 6.76422912[s]
 Temp_get = 23.4[degC]



----- PROCESSING PARAMETERS -----
 CPDPRG01 : 000000
 GPCP : 2.0 [Hz] : 0.0 [s]
 tpsrcoid3 : 0 [Hz] : 80 [Hz] : 100 [%]
 setofill : 1
 set : 1
 machinphase : TRUE
 PPM

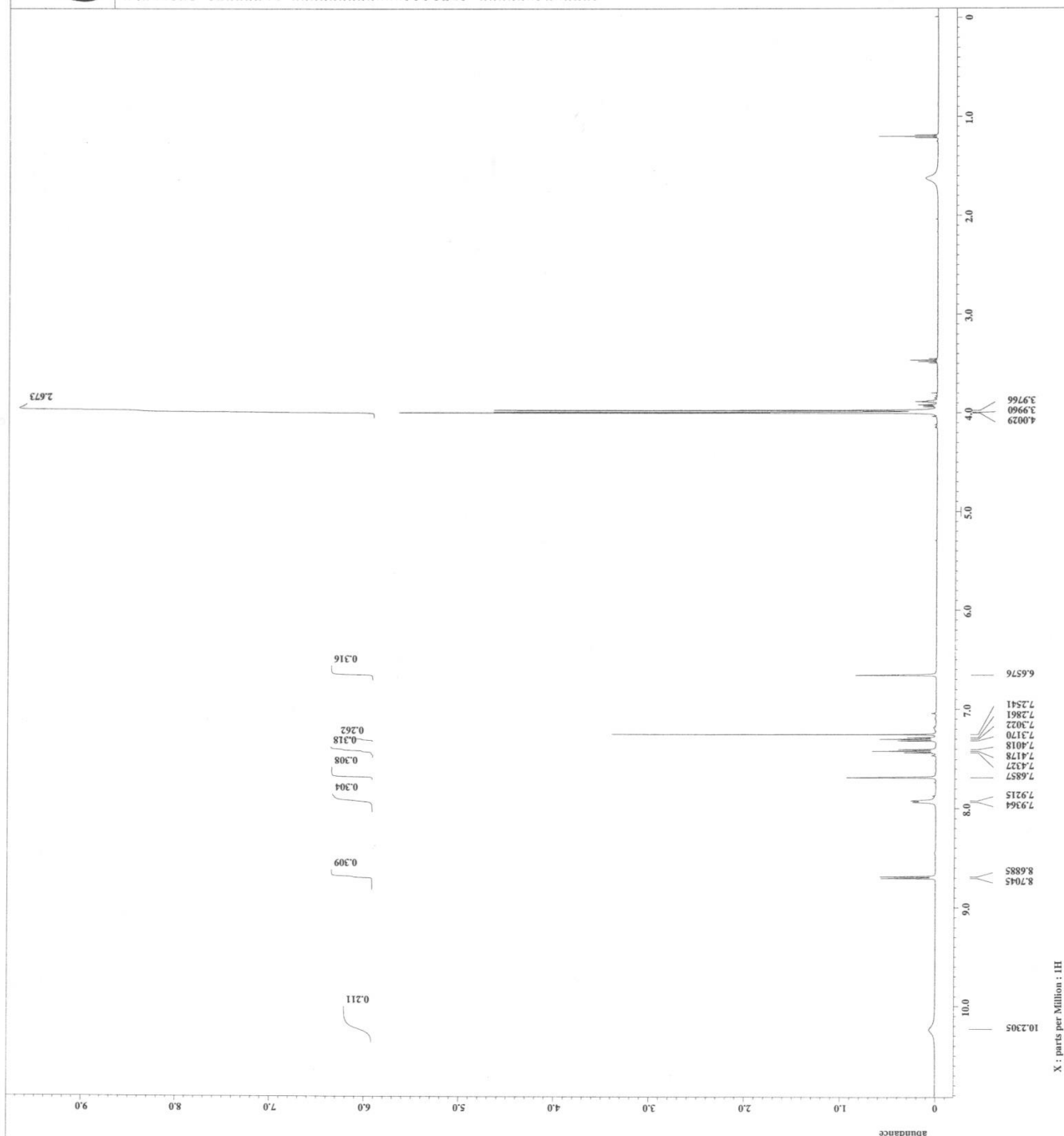
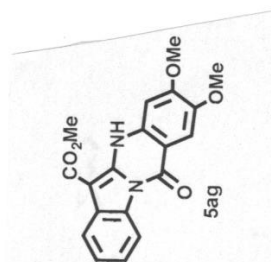
Derived from: TA160318-5-jdf

File Name : TA160318-8-jdf
 Author :
 Experiment : single_pulse_dec
 Sample ID : S857596
 Experiment : 160318-5
 Creation time : 13-MAR-2016 03:06:46
 Revision time : 22-MAR-2016 07:25:22
 Current time : 22-MAR-2016 07:26:00
 Comment : single pulse decouple
 Data format : 1D COMPLEX
 Dia_size : 12214
 Dia_unit : [mm]
 Dimensions :
 Site :
 Spectrometer : JEOL
 Field strength : 11.7473579 [T] (500 [MH]
 X_acq_time : 1.13361792 [s]
 X_resolution : 125.76529768 [kHz]
 X_offset : 100 [ppm]
 X_sweep : 2768
 X_resolution : 4
 X_sweep : 1.19959034 [Hz]
 X_resolution : 39.3081761 [kHz]
 X_offset : 500.15991521 [kHz]
 X_offset : 5.0 [ppm]
 X_offset : FALSE
 Total_scans : 51572.0
 X_90_width : 11.3 [us]
 X_acq_time : 0.83361792 [s]
 X_angle : 30 [deg]
 X_resolution : 3.76666667 [us]
 X_resolution : 21.318 [dB]
 X_resolution : 21.318 [dB]
 X_resolution : TRUE
 Initial_wait : 1 [s]
 Noe : TRUE
 Noe : TRUE
 Noe : TRUE
 Relaxation_delay : 2 [s]
 Relaxation_delay : 2.83361792 [s]
 Temp_set : 23.5 [C]



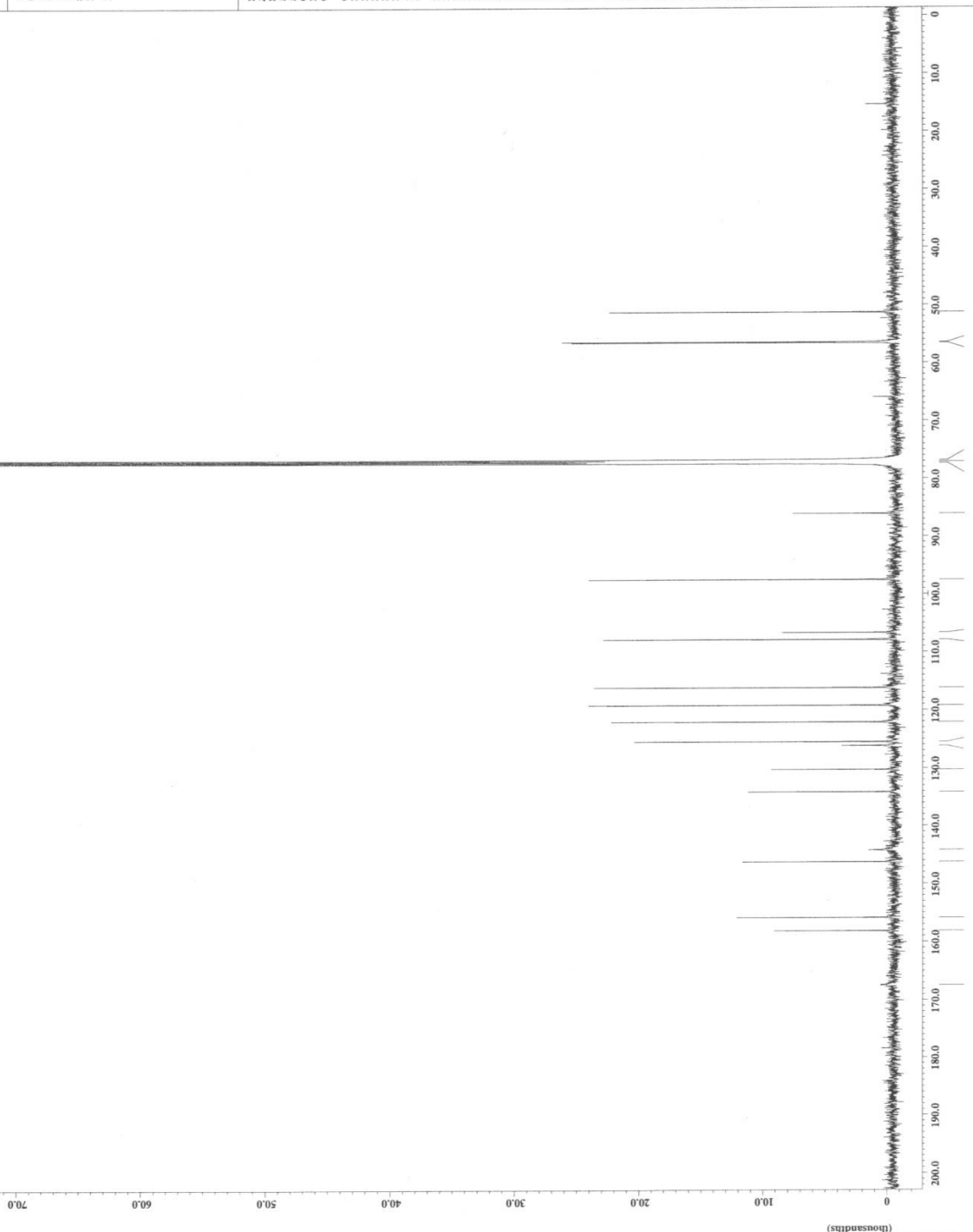
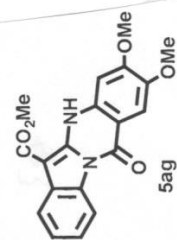
X : parts per Million : 13C

Filename	= Tal0373-4_jdf
Author	= dala
Experiment	= single_pulse_ox2
Experiment_id	= 1
Solvent	= CHLOROFORM-D
Creation_time	= 23-MAR-2016 08:10:19
Revision_time	= 23-MAR-2016 09:50:31
Current_time	= 23-MAR-2016 09:52:09
Content	= single_pulse
Data_format	= 1D_COMPLEX
File_name	= 13_07
File_title	= 13_07
Dia_units	= [ppm]
Dimensions	= KCA 500
Spectrometer	= DMZTAZ_NMR
Field_strength	= 13.62966421[s] (500.1M
X_acq_duration	= 1.76422912[s]
X_domain	= 1H
X_freq	= 495.13191398 [MHz]
X_offset	= 0.000000 [Hz]
X_resolution	= 0.566819 [Hz]
X_reso_scan	= 1
X_points	= 13.62966421 [Hz]
X_points	= 13.62966421 [Hz]
X_resolution	= 495.13191398 [MHz]
X_reso_scan	= 13 [ppm]
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.76422912[s]
X_offset	= 45 [deg]
X_resolution	= 6.3 [Hz]
X_reso_scan	= 8
X_points	= 8
X_freq	= 495.13191398 [MHz]
X_offset	= 5 [ppm]
X_resolution	= 1 [kHz]
X_reso_scan	= 8
X_points	= 13.6[s]
X_freq	= 1.



--- PROCESSING PARAMETERS ---
 acb1 : 1
 sedp : 2.0 [Hz] : 0.0 [s]
 trapdoid3 : 0 [Hz] : 80 [Hz] : 100 [Hz]
 sedf : 1
 fit : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: TAL60323-3.jdf

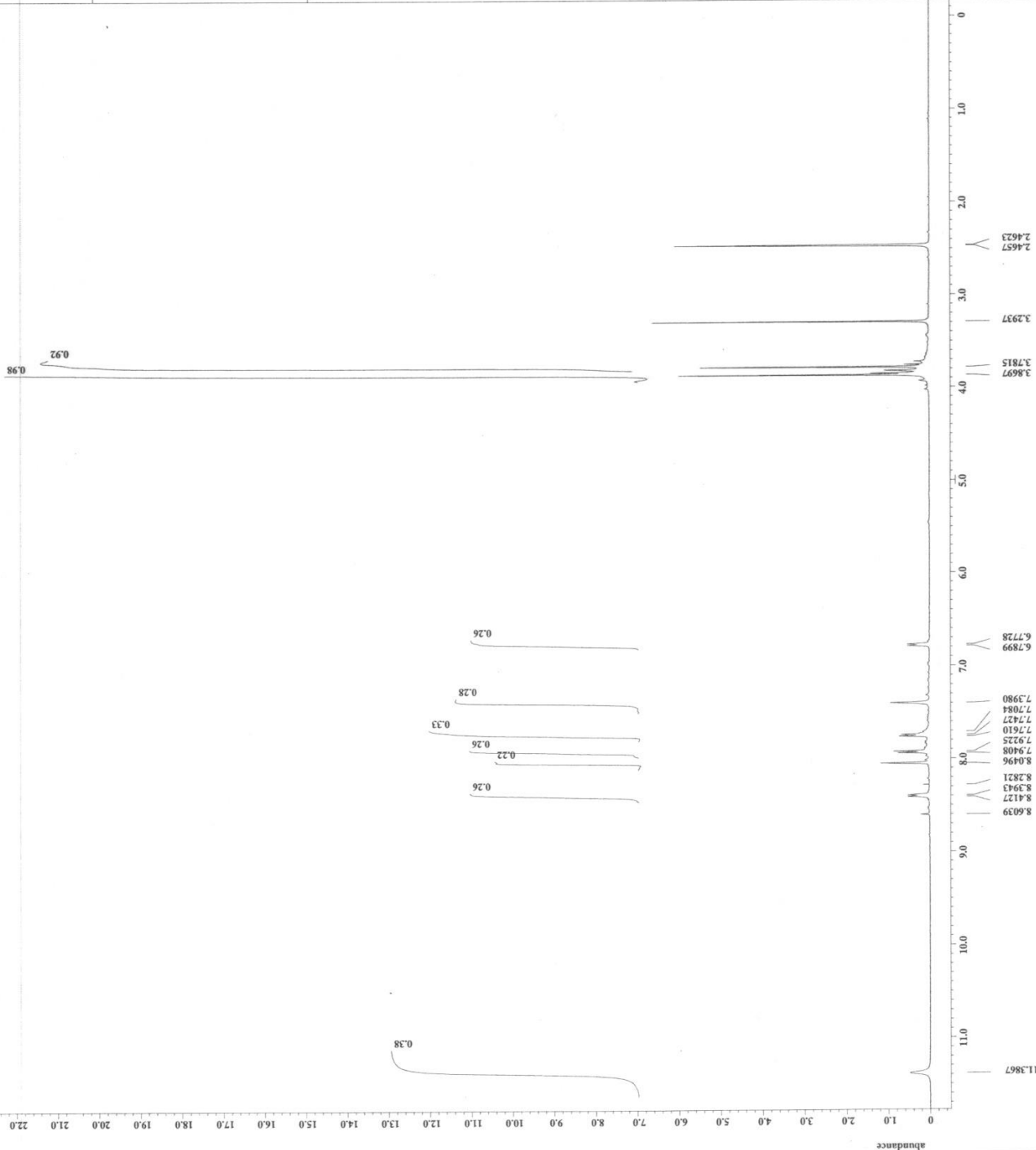
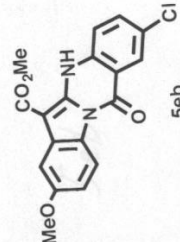
Filename = TAL60323-5.jdf
 Author =
 Experiment = single_pulse_dec
 Sample_id = S8573232
 Date_ime = 2016-03-19 02:18:39
 Creation_time = 19-MAR-2016 02:18:39
 Revision_time = 24-MAR-2016 08:27:39
 Current_time = 24-MAR-2016 08:31:09
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_units = [ppm]
 Dimensions = X
 Site = MCA500
 Spectrometer = JEOL_JNM
 Field_strength = 11.7473575 [T] (500 [MHz])
 X_acq_duration = 0.83361792 [s]
 X_freq = 125.76529768 [MHz]
 X_offset = 100 [ppm]
 X_points = 27768
 X_resolution = 1.19959634 [Hz]
 X_sweep = 39.3081761 [MHz]
 X_spin = 500.15991521 [MHz]
 Xr_offset = 5.0 [ppm]
 Clipped = FALSE
 Acq_return = 20923
 Total_scans = 20923
 X30_width = 11.3 [us]
 X30_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 5.2 [dB]
 X30_delay = 11.318 [us]
 Xr_atn_dec = 21.318 [dB]
 Xr_atn_poe = 21.318 [dB]
 Xr_noise = WALTZ
 Xr_delay = 1 [s]
 Xr_wait = 1 [s]
 Noe_time = TRUE
 Noe_time_in = 2 [s]
 Relaxation_delay = 2 [s]
 Repetition_time = 2.83361792 [s]
 Temp_set = 24 [degC]



----- PROCESSING PARAMETERS -----
 GC.DA160428-2-2.jdf
 Date: 2016-05-03 13:08:34
 Time: 13:08:34
 User: jk
 Machine: TRUE
 PPM

Derived from: DA160428-2.jdf

=====
 File Name: DA160428-2-2.jdf
 Experiment: single_pulse.ex2
 Sample ID: S8340050
 Date: 2016-05-03 13:08:34
 Revision: 1
 Current Time: 2-MAY-2016 13:08:34
 Comment: single_pulse
 Data Format: 1D COMPLEX
 Data Size: 13107
 Data Units: [ppm]
 Dimensions: X
 Site: ECA505
 Spectrometer: ECA505_NMR
 Field Strength: 11.7473579 [T] 500 [MH]
 X1: 11.7473579 [T] 500 [MH]
 X2: 1H 4587904 [a]
 X3: 500.15991521 [MHz]
 X4: 5.0 [ppm]
 X5: 1.6384
 X6: 0.5727737 [Hz]
 X7: 9.38438438 [kHz]
 X8: 500.15991521 [MHz]
 X9: 5.0 [ppm]
 X10: 300.15991521 [MHz]
 X11: 5.0 [ppm]
 X12: FALSE
 Mod Return: 1
 Total Scans: 8
 X13: 11.7473579 [T] 500 [MH]
 X14: 11.7473579 [T] 500 [MH]
 X15: 45 [deg]
 X16: 3.4 [dB]
 X17: 0 [us]
 X18: Off
 X19: Off
 X20: FALSE
 X21: 1 [us]
 X22: 60
 X23: 5 [s]
 X24: 6.74587904 [a]
 X25: 22.1 [deg]



X : parts per Million : 1H

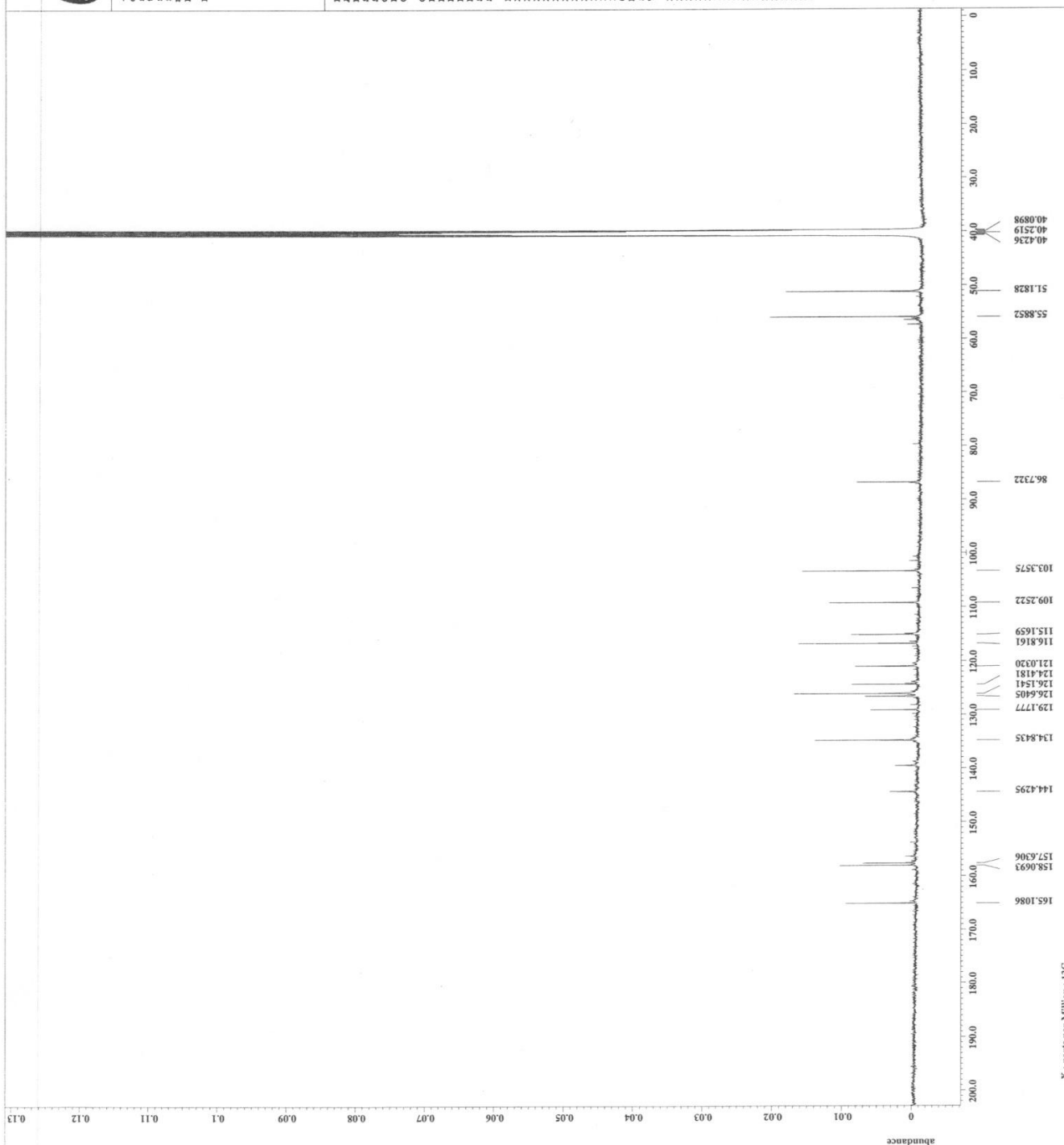
```

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

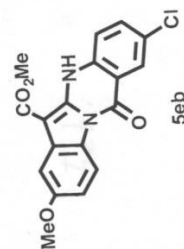
```

Derived from: TA160428-50Me-5C1-1.jdf

Filename	= D:\04128-5086-5C1-2...
Author	= data
Experiment	= single_pulse_dec
Sample_id	= DMSO-D6
Solvent	= DMSO-D6
Creation_time	= 27-APR-2016 03:01:35
Revision_time	= 27-APR-2016 03:01:35
Creation_time	= 27-APR-2016 03:01:35
Current_time	= 27-APR-2016 03:01:35
Comment	= single_pulse decouple
Data_format	= 13C
File_name	= 13C
Dir_title	= 13C
Dir_name	= 13C
Dir_path	= 13C
Dimensions	= 1D
Spectrometer	= ECA300
Field_strength	= DELTA2_NMR
Acq_duration	= 11.74755973 [s] 650 [MHz]
Acq_time	= 0.836372 [s]
Acq_date	= 13C
Freq	= 125.7629768 [MHz]
Resolution	= 125.7629768 [MHz]
Points	= 32768
Prescans	= 4
Resolution	= 1.19559034 [Hz]
Ir_fdomain	= 135.7681762 [MHz]
Ir_freq	= 150.15994521 [MHz]
Ir_offset	= 5.0 [ppm]
Mod_setup	= 1 pulse
Scans	= 17951
Total_scans	= 17951
X90_width	= 11.3 [us]
X90_time	= 0.836372 [s]
X90_date	= 13C
Xpulse	= 5 [dB]
Ypulse	= 3.76666667 [us]
Y1_pulse	= 21.31 [dB]
Y2_pulse	= 21.31 [dB]
Y3_pulse	= 21.31 [dB]
Y4_pulse	= 21.31 [dB]
Y5_pulse	= 21.31 [dB]
Y6_pulse	= 21.31 [dB]
Y7_pulse	= 21.31 [dB]
Y8_pulse	= 21.31 [dB]
Y9_pulse	= 21.31 [dB]
Y10_pulse	= 21.31 [dB]
Y11_pulse	= 21.31 [dB]
Y12_pulse	= 21.31 [dB]
Y13_pulse	= 21.31 [dB]
Y14_pulse	= 21.31 [dB]
Y15_pulse	= 21.31 [dB]
Y16_pulse	= 21.31 [dB]
Y17_pulse	= 21.31 [dB]
Y18_pulse	= 21.31 [dB]
Y19_pulse	= 21.31 [dB]
Y20_pulse	= 21.31 [dB]
Y21_pulse	= 21.31 [dB]
Y22_pulse	= 21.31 [dB]
Y23_pulse	= 21.31 [dB]
Y24_pulse	= 21.31 [dB]
Y25_pulse	= 21.31 [dB]
Y26_pulse	= 21.31 [dB]
Y27_pulse	= 21.31 [dB]
Y28_pulse	= 21.31 [dB]
Y29_pulse	= 21.31 [dB]
Y30_pulse	= 21.31 [dB]
Y31_pulse	= 21.31 [dB]
Y32_pulse	= 21.31 [dB]
Y33_pulse	= 21.31 [dB]
Y34_pulse	= 21.31 [dB]
Y35_pulse	= 21.31 [dB]
Y36_pulse	= 21.31 [dB]
Y37_pulse	= 21.31 [dB]
Y38_pulse	= 21.31 [dB]
Y39_pulse	= 21.31 [dB]
Y40_pulse	= 21.31 [dB]
Y41_pulse	= 21.31 [dB]
Y42_pulse	= 21.31 [dB]
Y43_pulse	= 21.31 [dB]
Y44_pulse	= 21.31 [dB]
Y45_pulse	= 21.31 [dB]
Y46_pulse	= 21.31 [dB]
Y47_pulse	= 21.31 [dB]
Y48_pulse	= 21.31 [dB]
Y49_pulse	= 21.31 [dB]
Y50_pulse	= 21.31 [dB]
Y51_pulse	= 21.31 [dB]
Y52_pulse	= 21.31 [dB]
Y53_pulse	= 21.31 [dB]
Y54_pulse	= 21.31 [dB]
Y55_pulse	= 21.31 [dB]
Y56_pulse	= 21.31 [dB]
Y57_pulse	= 21.31 [dB]
Y58_pulse	= 21.31 [dB]
Y59_pulse	= 21.31 [dB]
Y60_pulse	= 21.31 [dB]
Y61_pulse	= 21.31 [dB]
Y62_pulse	= 21.31 [dB]
Y63_pulse	= 21.31 [dB]
Y64_pulse	= 21.31 [dB]
Y65_pulse	= 21.31 [dB]
Y66_pulse	= 21.31 [dB]
Y67_pulse	= 21.31 [dB]
Y68_pulse	= 21.31 [dB]
Y69_pulse	= 21.31 [dB]
Y70_pulse	= 21.31 [dB]
Y71_pulse	= 21.31 [dB]
Y72_pulse	= 21.31 [dB]
Y73_pulse	= 21.31 [dB]
Y74_pulse	= 21.31 [dB]
Y75_pulse	= 21.31 [dB]
Y76_pulse	= 21.31 [dB]
Y77_pulse	= 21.31 [dB]
Y78_pulse	= 21.31 [dB]
Y79_pulse	= 21.31 [dB]
Y80_pulse	= 21.31 [dB]
Y81_pulse	= 21.31 [dB]
Y82_pulse	= 21.31 [dB]
Y83_pulse	= 21.31 [dB]
Y84_pulse	= 21.31 [dB]
Y85_pulse	= 21.31 [dB]
Y86_pulse	= 21.31 [dB]
Y87_pulse	= 21.31 [dB]
Y88_pulse	= 21.31 [dB]
Y89_pulse	= 21.31 [dB]
Y90_pulse	= 21.31 [dB]
Y91_pulse	= 21.31 [dB]
Y92_pulse	= 21.31 [dB]
Y93_pulse	= 21.31 [dB]
Y94_pulse	= 21.31 [dB]
Y95_pulse	= 21.31 [dB]
Y96_pulse	= 21.31 [dB]
Y97_pulse	= 21.31 [dB]
Y98_pulse	= 21.31 [dB]
Y99_pulse	= 21.31 [dB]
Y100_pulse	= 21.31 [dB]
Y101_pulse	= 21.31 [dB]
Y102_pulse	= 21.31 [dB]
Y103_pulse	= 21.31 [dB]
Y104_pulse	= 21.31 [dB]
Y105_pulse	= 21.31 [dB]
Y106_pulse	= 21.31 [dB]
Y107_pulse	= 21.31 [dB]
Y108_pulse	= 21.31 [dB]
Y109_pulse	= 21.31 [dB]
Y110_pulse	= 21.31 [dB]
Y111_pulse	= 21.31



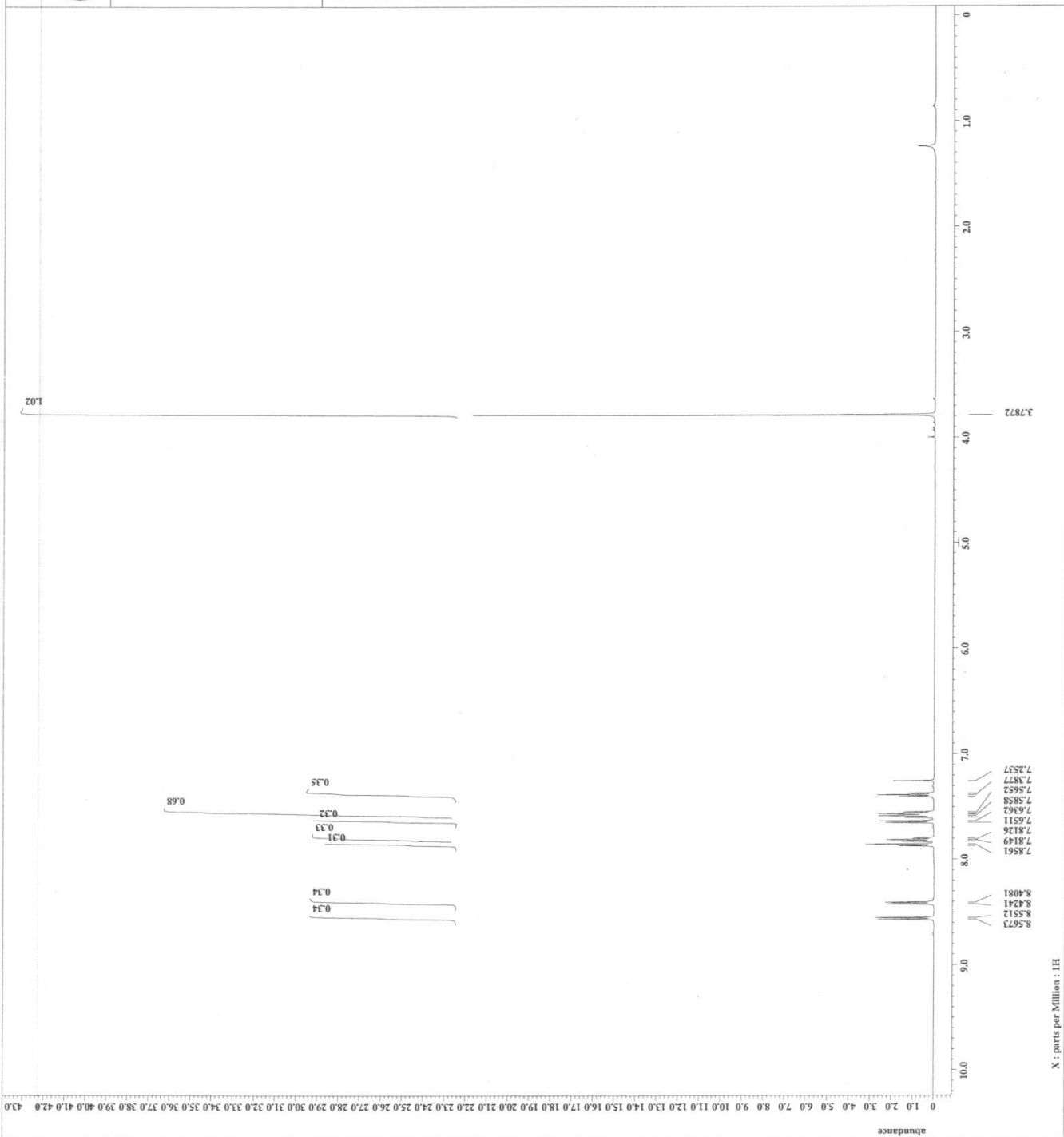
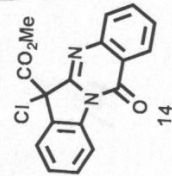
X : parts per Million : 13C





----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
freq : 500.13591521 [MHz]
temp : 23 [C]
traprod3 : 0 [s] : 80 [s] : 100 [s]
zerofill : 1
fft : 1 : TRUE : TRUE
machinename :
ppm
Derived from: TAL60225-1.jdf

Filename = TAL60225-1.jdf
Sample =
Experiment = single_pulse.exe
Sample_id = SM376057
Solvent = CHLOROFORM-D
Acq_date = 25-FEB-2016 10:31:44
Acq_time = 25-FEB-2016 10:31:38
Revision_time = 25-FEB-2016 10:32:55
Current_time =
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dimensions = X
Spectrometer = ECA500
Site = DELTA_NMR
Field_strength = 11.7473579 [T] : 500 [MH]
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_offset = 500.15991521 [MHz]
X_points = 5.0 [ppm]
X_prescan = 16384
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 500.15991521 [MHz]
Irr_points = 5.0 [ppm]
Irr_sweep = 9.38438438 [kHz]
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.8 [us]
X_acq_time = 1.74587904 [s]
X_delay = 4.0 [us]
X_pulse = 3.4 [us]
X_pulse = 5.9 [us]
Irr_mode = Off
Irr_delay = Off
Data_preset = FALGE
Initial_wait = 1 [s]
Recvr_gain = 46
Repetition_delay = 3.0 [s]
Repetition_time = 6.74587904 [s]
Temp_get = 23 [C]



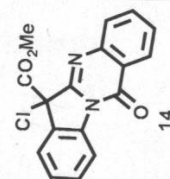
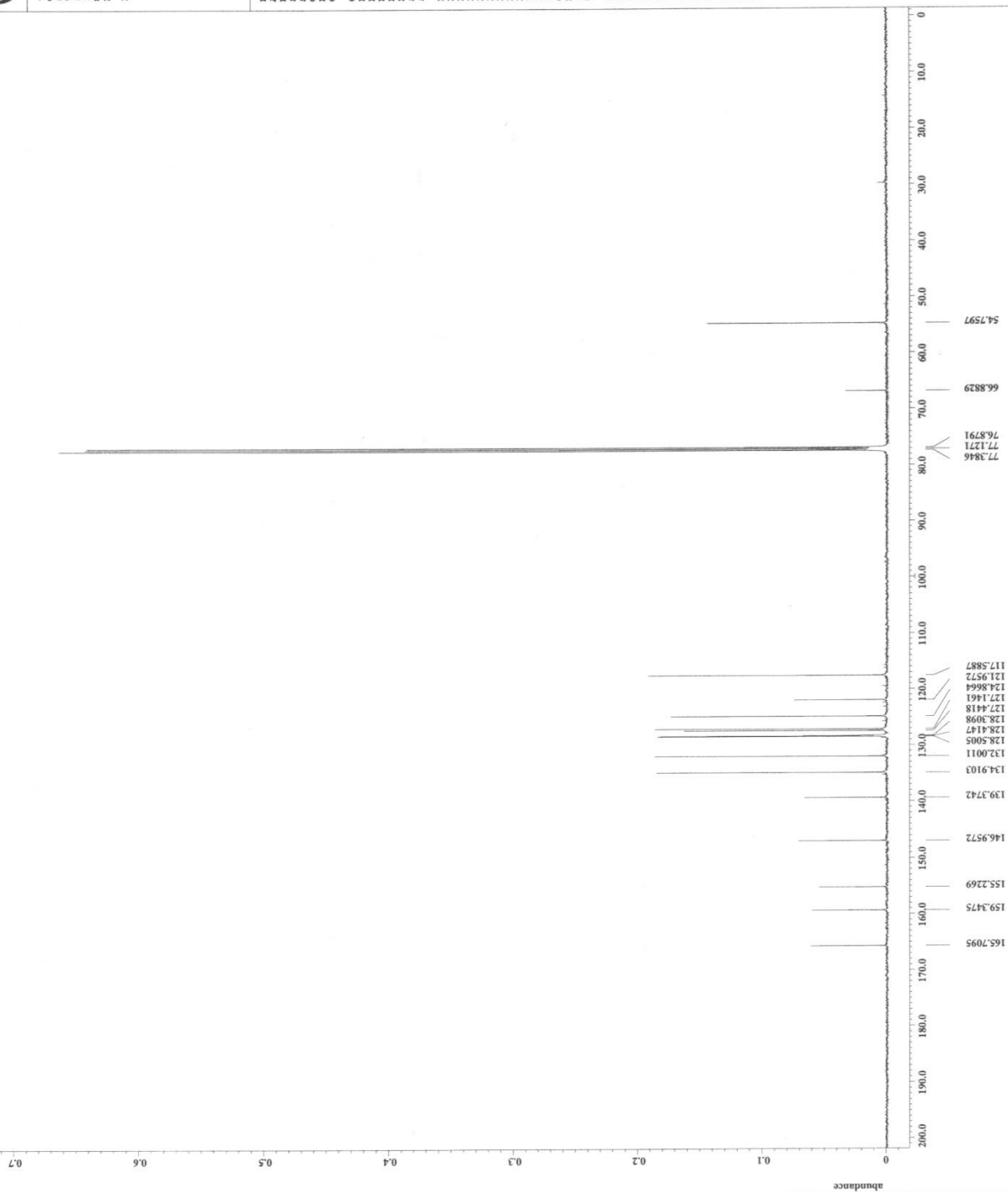
```

----- PROCESSING PARAMETERS -----
dc balance : 0 : FALSE
semp : 2.0[Hz] : 0.0[s]
traperrorid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fit : 1 : TRUE
machinephase
ppm

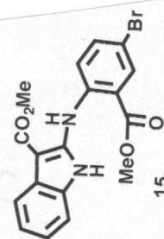
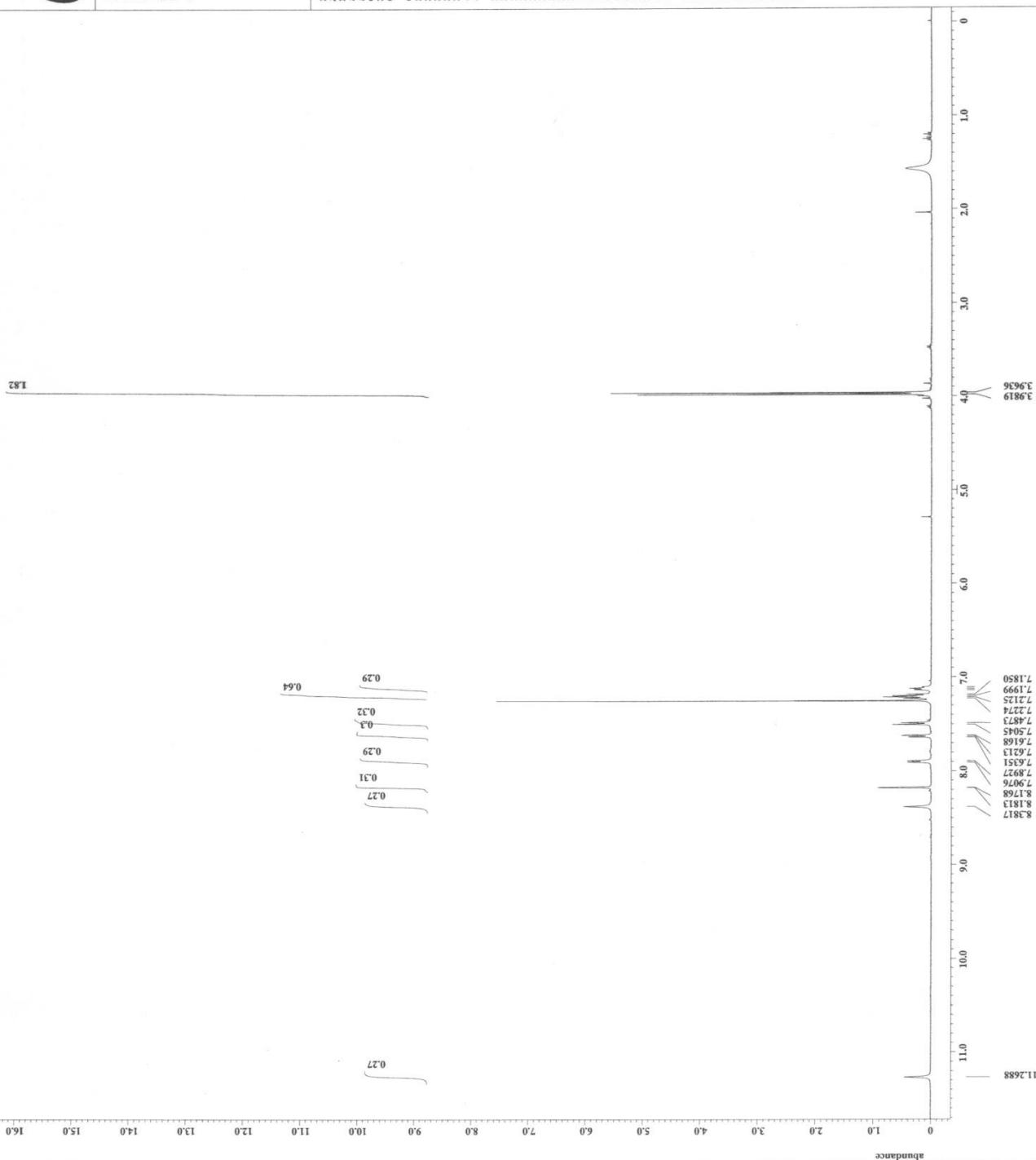
```

Derived from: TA160225-2.jdf

Filenames	= RA602029S_3.jdf
Author	= single_pulse_dec
Experiment	= RA602029S-D
ObservedTime	= 22-FEB-2016 16:00:09
Creation_time	= 25-FEB-2016 12:09:04
Creation_date	= 25-FEB-2016 13:11:17
Current	= single pulse decouple
Comment	= ID COMPLEX
Data format	= 13C
Spin file	= 13C
Spin units	= [ppm]
Dimensions	= 4
Spectrometer	= KAS90
Field_strength	= 11.747850 [G] (500 [MHz])
Acq_start	= 0.936572 [s]
X_domain	= 13C
X_center	= 135.7652768 [MHz]
X_points	= 32768
X_resolution	= 1.1995904 [Hz]
Y_domain	= 21.308769 [kHz]
Y_center	= 50.159994521 [MHz]
Y_offset	= 5.0 [ppm]
Hf_offset	= 1.0 [ppm]
Noise	= 2223
Scans	= 2223
Total_scans	= 11.3 [us]
X90_width	= 0.83661792 [s]
X_acq_time	= 5 [ms]
X_wait	= 5 [ms]
X_pulse	= 3.76666667 [us]
Ir_rst_dec	= 21.318 [dB]
Ir_rst_amp	= NAU72
Ir_noise	= TRUE
Decoupling	= 1[s]
Initial_wait	= 5[s]
Noise	= 54
Recv_gain	= 23.7 [dBS]
Relaxation_delay	= 23.7 [s]
Relaxation_time	= 23.7 [s]
Temp_set	= 23.7 [dBS]



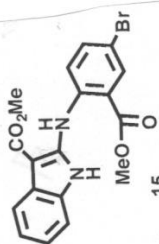
X : parts per Million : 13C

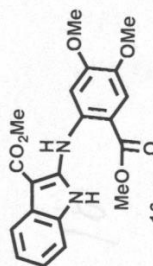


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```
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
freq       : 0.2 [Hz] : 0.0[s]
taper      : 0.0 [s] : 0.0[s]
arrazoid   : 0 [%] : 80[%] : 100[%]
zerofill   : 1
fft        : 1 : TRUE : TRUE
machinphase
ppm
Derived from: TAL60314-5.jdf
```

[illegible]





Filename	"data
Author	"single_pulse_dec
Experiment	"DMO-d4
Solvent	"DMO-d4
Creation_time	"24-MAR-2016 06:51:56
Creation_time	"24-MAR-2016 08:05:56
Current_time	"24-MAR-2016 08:19:19
Content	"single pulse decouple 1D COMPLEX 13C X3,4 X [ppm] X X3, 500 SPECTROSCOPY DMT/32_NMR
Spctral_width [Hz]	13.6292621 [7] 500 [M]
Acq_duration [s]	0.139288 [0.13]
X_domain	13C
X_freq [MHz]	125.760305 [125.76]
X_resolution [ppm]	14.5010059 [MHz]
X_points	144
X_rescans	32764
X_resolution	4
Y_resolution [Hz]	1.1920222 [Hz]
Y_domain	13C
Y_freq [MHz]	125.76025 [MHz]
Y_resolution [ppm]	495.13191398 [MHz]
Y_offset [ppm]	5 [ppm]
Y_return	1
Mode	1DUSE
Scans	10669
Total_scans	10669
X30_width [s]	0.0388608 [s]
X30_acq_time	0.0388608 [s]
X30_pulse	9.81 [us]
X_pulse	9.81 [us]
X30_gain	3.5 [us]
X_gain	3.5 [us]
Y30_width [s]	20.86935 [s]
Y30_acq_time	20.86935 [s]
Y30_pulse	10.0 [us]
Y30_gain	10.0 [us]
Y30_noise	NAUTZ
Decoupling	"TUS
Initial_wait [s]	1 [s]
Initial_wait	2181
Acq_time	2181
Recv_time	60
Relaxation_delay [s]	21.818608 [s]
Relaxation_delay	21.818608 [s]
Relax_time	21.8192 [s]
Relax_time	21.8192 [s]

