

Supporting Information

Hydrolysis of Amides to Carboxylic Acids Catalyzed by Nb₂O₅

S. M. A. Hakim Siddiki,^{†*} Md. Nurnobi Rashed,[†] Abeda Sultana Touchy,[†] Md. A. R. Jamil,[†]
Yuan Jing,[†] Takashi Toyao,^{†,‡} Zen Maeno,[†] Ken-ichi Shimizu^{*†,‡}

[†] Institute for Catalysis, Hokkaido University, N-21, W-10, Sapporo 001-0021, Japan

[‡] Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Katsura, Kyoto
615-8520, Japan.

*Corresponding authors

S. M. A. Hakim Siddiki, Ken-ichi Shimizu

E-mail: hakim@cat.hokudai.ac.jp, kshimizu@cat.hokudai.ac.jp

Experimental:

General

Commercially available inorganic and organic compounds were purchased from TCI (Tokyo Chemical Industry), Sigma Aldrich, Wako Pure Chemical Industries, Kishida Chemical, or Mitsuwa Chemicals and were used without further purification. The GC (Shimadzu GC-14B) and GCMS (Shimadzu GCMS-QP2010) analyses were conducted using an Ultra ALLOY capillary column UA⁺-1 (Frontier Laboratories Ltd.) with N₂ and He as carrier gases. ¹H and ¹³C NMR spectra were recorded at ambient temperature on JEOL-ECX 600 and 400 instruments operating at 600.17 and 150.92 MHz and at 395.88 and 99.54 MHz respectively with dimethyl sulfoxide (DMSO) as an internal standard.

Catalyst preparation

Different Nb₂O₅ samples were prepared by calcination of Nb₂O₅·*n*H₂O (HY-340, provided by CBMM, Brazil) at 200 °C, 500 °C, 700 °C, and 1000 °C for 3h in air prior to use. CeO₂, supplied from Daiichi Kigenso Kagaku Kogyo Co., Ltd (Type A), was calcined at 600 °C for 3 h. TiO₂ (JRC-TIO-8) and MgO (JRC-MGO-3) were supplied by the Catalysis Society of Japan. γ-Al₂O₃ was prepared by calcination of γ-AlOOH (Catapal B Alumina, Sasol) at 900 °C for 3 h. SiO₂ (Q-10) was supplied by Fuji Silysia Chemical Ltd. ZnO was prepared by calcination (*T* = 500 °C, *t* = 3 h) of Zn(OH)₂ (Kishida Chemical). ZrO₂ was prepared by calcining Zr(OH)₄ at 773 K for 3 h, which was made *via* hydrolysis of Y(NO₃)₃·6H₂O, ZrO(NO₃)₂·2H₂O with an aqueous NH₄OH solution. SnO₂ was prepared from H₂SnO₃ (Kojundo Chemical Laboratory Co., Ltd.) by calcination at 500 °C for 3 h. CaO was prepared by calcination of Ca(OH)₂ (Kanto Chemical) at 500 °C for 3 h. La₂O₃, Ce(NO₃)₄, *p*-toluenesulfonic acid, and H₂SO₄ were supplied by Wako Pure Chemical Industries, Japan. The Sc(OTf)₃ (>98%) was obtained from TCI Co. Ltd., and Zr(SO₄)₄·4H₂O (≥99%) was supplied from Alfa Aesar, Ward Hill, China. Montmorillonite K10 clay (mont. K10), sulfonic resin Nafion-SiO₂ composite, and ammonium niobate(V) oxalate hydrate (C₄H₄NNbO₉·*x*H₂O) were purchased from Sigma-Aldrich.

Catalyst characterization

X-ray diffraction (XRD; Rigaku MiniFlex) patterns of the powdered catalysts were recorded using Cu-Kα radiation ($\lambda = 1.5418 \text{ \AA}$). The N₂ adsorption measurements were obtained over AUTOSORB 6AG (Yuasa Ionics Co.). X-ray photoelectron spectroscopy (XPS) of the catalysts was performed using a JEOL JPS-9010MC spectrometer (Mg-Kα irradiation). Binding energies were calibrated with respect to C_{1s} at 285.0 eV. Inductively coupled plasma-atomic emission spectroscopy (ICP-AES) analysis was done with a Shimadzu ICPE-9000 instrument to investigate the heterogeneous nature of Nb₂O₅ catalysts.

IR studies

In situ IR spectra were recorded using a JASCO FT/IR-4200 with an MCT (mercury-cadmium-telluride) detector. The Nb₂O₅ sample (40 mg) was pressed to obtain a self-supporting pellet ($\phi = 2$ cm), which was placed in the quartz IR cell with CaF₂ windows connected to a conventional gas flow system. Spectra were obtained by accumulating 15 scans at a resolution of 4 cm⁻¹. A reference spectrum taken at the adsorption measurement temperature (120 °C) under He flow was subtracted from each spectrum.

For acetamide adsorption experiments, the sample pellet was heated under He flow (100 cm³ min⁻¹) at 300 °C for 0.5 h prior to the measurement. After cooling to 120 °C under the He flow, 1 μ L acetamide was injected into each sample through a line which was preheated at ca. 200 °C to vaporize it.

For pyridine adsorption experiments, the sample was activated at 200 °C for 0.5 h under He flow (100 cm³ min⁻¹) and then cooled down to 120 °C. Subsequently, 1 μ L pyridine was introduced. The amount of adsorbed probe molecule was determined using the integrated area of bands typical of the coordinated (Lewis) or protonated (Brønsted) forms at 1445 and 1540 cm⁻¹, respectively, using previously determined molar absorption coefficients.¹

Typical procedure for catalytic reactions

Amide **1a** (1 mmol), water (5 mmol), and a magnetic stirrer bar were placed in a reaction tube followed by addition of N₂ through the septum inlet. The standard amount of catalyst used was 50 mg. The temperature controller was set at 120 °C to maintain reflux conditions during the reaction. Yields of products were determined by GC with *n*-dodecane as the internal standard. GC sensitivities were estimated using commercial compounds or isolated products. In substrate scope studies, products were isolated using column chromatography on silica gel 60 (spherical, 40–100 μ m, Kanto Chemical Co. Ltd.) using hexane/ethyl acetate (10:1 to 16:1, v/v) as the eluting solvent, followed by ¹H and ¹³C NMR spectroscopy in combination with GC-MS equipped with the same column as that used for GC-FID analyses. For recycling experiments, after each catalytic cycle, 2-propanol (3 mL) was added into the reaction mixture. The catalyst was separated and washed twice with acetone (3 mL) followed by water (3 mL). The catalyst was then dried at 110 °C for 5 h and used.

Supplementary results:

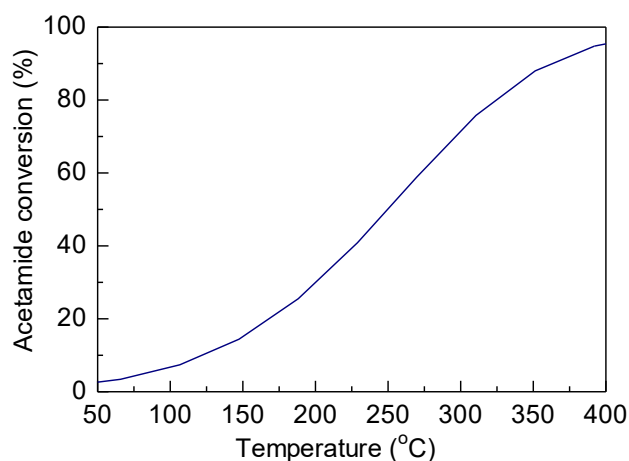


Figure S1. Thermodynamic equilibrium of acetamide conversion in hydrolysis of acetamide to acetic acid calculated using HSC Chemistry 9.0 software. The reaction $C_2H_5NO + H_2O(l) = C_2H_4O_2(a) + NH_3(a)$ was examined with a water/acetamide ratio = 5.

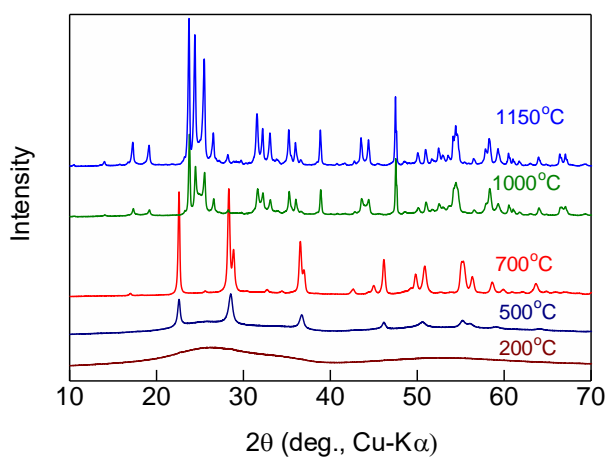


Figure S2. XRD patterns of Nb_2O_5 catalysts calcined at different temperatures.

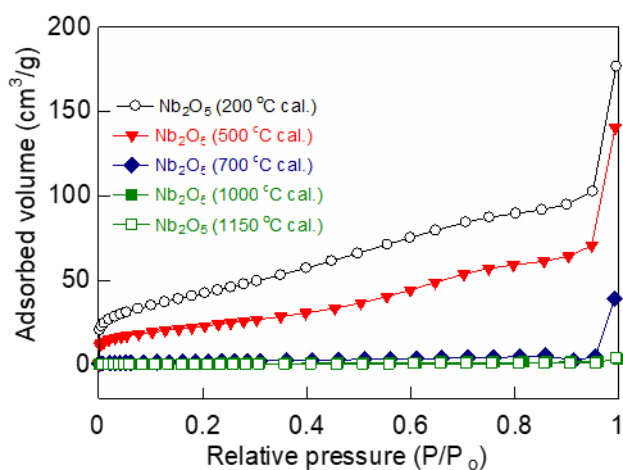


Figure S3. N_2 adsorption isotherms of Nb_2O_5 catalysts calcined at different temperatures.

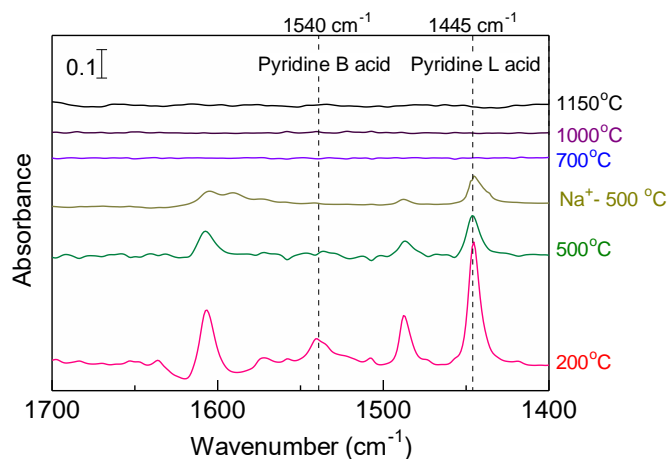


Figure S4. IR spectra of pyridine adsorption on Nb_2O_5 catalysts calcined at different temperatures. The spectra were measured at 200 °C.

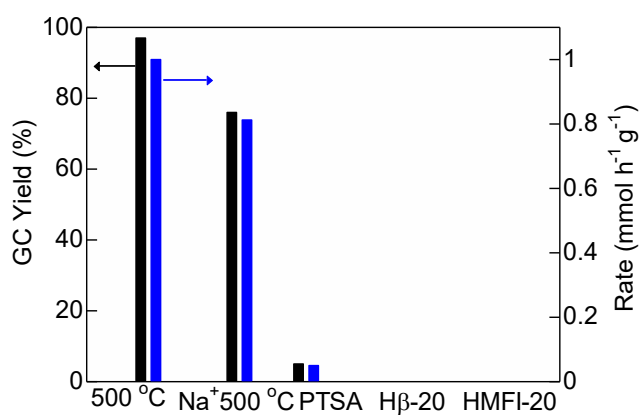
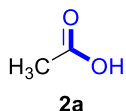


Figure S5. Comparison of the role of Lewis and Brønsted acid sites of catalysts on hydrolysis of acetamide. Reaction conditions: acetamide 1 mmol, water 5 mmol, catalysts 50 mg, $T = 120\text{ °C}$, $t = 20\text{ h}$ (final yield determination), 2 h (initial rate determination).

NMR and GC/MS analyses:

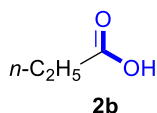
^1H and ^{13}C NMR spectra of the products were assigned and confirmed by literature values. ^1H and ^{13}C NMR spectra were recorded at ambient temperature on a JEOL-ECX 600 instrument operating at 600.17 MHz and 150.92 MHz, respectively, and a JEOL-ECX 400-2 instrument operating at 399.78 MHz and 100.52 MHz, respectively. Abbreviations used in the NMR experiments: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. GC-MS spectra were obtained using a Shimadzu QP2010 instrument.

Acetic acid:²



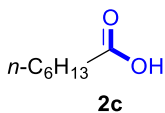
Yield 91%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.94 (s, 1H), 1.89 (s, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 172.18, 21.12; GC-MS m/z : 60.05.

Propionic acid:³



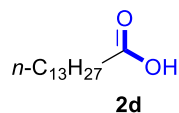
Yield 90%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.95 (s, 1H), 2.22-2.18 (m, 2H), 0.98 (t, $J=7.56$ Hz, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 175.27, 26.94, 9.13; GC-MS m/z : 74.05.

Hexanoic acid:⁴



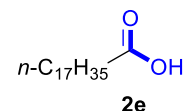
Yield 84%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.96 (s, 1H), 2.18 (t, $J=7.56$ Hz, 2H), 1.51-1.42 (m, 2H), 1.32-1.19 (m, 4H), 0.85 (t, $J=7.08$ Hz, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 174.52, 33.65, 30.80, 24.21, 21.87, 13.84; GC-MS m/z : 116.15.

Tetradecanoic acid:⁵



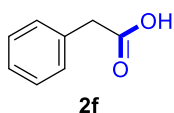
Yield 77%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.96 (s, 1H), 2.17 (t, $J=7.56$ Hz, 2H), 1.48-1.42 (m, 2H), 1.29-1.19 (m, 20H), 0.85 (t, $J=7.05$ Hz, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 174.50, 33.67, 31.31, 30.81, 29.03 (C \times 2), 28.92, 28.75, 28.72 (C \times 2), 28.56, 24.50, 22.11, 13.96; GC-MS m/z : 228.35.

Heptadecanoic acid:⁶



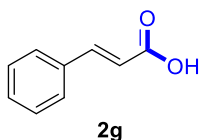
Yield 86%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.68 (s, 1H), 2.18 (t, J =7.56 Hz, 2H), 1.54-1.49 (m, 2H), 1.34-1.19 (m, 28H), 0.86 (t, J =6.87 Hz, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 173.85, 33.40, 30.90, 30.80, 28.61 (C \times 2), 28.49 (C \times 2), 28.31 (C \times 2), 28.26 (C \times 2), 28.21 (C \times 2), 24.17, 21.65, 13.42; GC-MS m/z : 270.45.

Phenylacetic acid:⁷



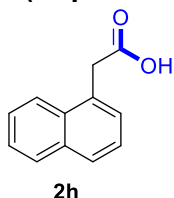
Yield 88%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.32 (s, 1H), 7.30 (t, J =7.44 Hz, 2H), 7.27-7.21 (m, 3H), 3.56 (s, 2H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 172.75, 135.06, 129.40 (C \times 2), 128.26 (C \times 2), 126.61, 40.72; GC-MS m/z : 136.15.

3-Phenyl-acrylic acid:⁸



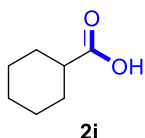
Yield 84%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.46 (s, 1H), 7.65 (t, J =8.22 Hz, 2H), 7.62 (t, J =8.12 Hz, 1H), 7.40-7.361 (m, 3H), 6.54 (t, J =8.012 Hz, 1H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 167.80, 144.09, 134.39, 130.32, 129.02 (C \times 2), 128.31 (C \times 2), 119.38; GC-MS m/z : 148.15.

2-(Naphthalen-1-yl)acetic acid:⁸



Yield 83%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 12.43 (s, 1H), 7.97 (d, J =8.10 Hz, 1H), 7.92 (d, J =8.04 Hz, 1H), 7.84 (d, J =8.04 Hz, 1H), 7.58-7.351 (m, 2H), 7.48-7.34 (m, 2H), 4.04 (s, 2H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 172.78, 133.34, 131.89, 131.69, 128.46, 128.01, 127.40, 126.18, 125.72, 125.54, 124.04, 38.50; GC-MS m/z : 186.20.

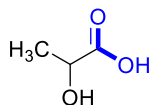
Cyclohexanecarboxylic acid:⁵



Yield 95%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.94 (s, 1H), 2.20-2.15 (m, 1H), 1.82-1.76 (m, 2H), 1.68-1.62 (m, 2H), 1.59-1.531 (m, 2H), 1.33-1.14 (m, 5H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 176.75,

42.28, 28.73, 25.52 (C×2), 25.01 (C×2); GC-MS m/z: 128.15.

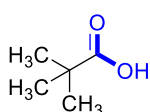
2-Hydroxypropanoic acid:⁹



2j

Yield 88%; ¹H NMR (600.17 MHz, DMSO-d₆): δ 12.35 (br s, 1H), 5.24 (br s, 1H), 4.09-4.05 (m, 1H), 1.26 (d, *J* = 6.60 Hz, 3H); ¹³C NMR (150.92 MHz, DMSO-d₆) δ 177.42, 66.83, 21.51; GC-MS m/z: 90.10.

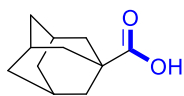
Propionic acid:¹⁰



2k

Yield 91%; ¹H NMR (600.17 MHz, DMSO-d₆): δ 12.01 (br s, 1H), 1.10 (s, 9H); ¹³C NMR (150.92 MHz, DMSO-d₆) δ 179.37, 37.92, 27.01 (C×3); GC-MS m/z: 102.15.

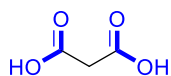
Adamantane-1-carboxylic acid:¹¹



2l

Yield 83%; ¹H NMR (600.17 MHz, DMSO-d₆): δ 11.97 (s, 1H), 1.94 (br s, 9H), 1.78 (s, 6H), 1.68-1.62 (m, 5H); ¹³C NMR (150.92 MHz, DMSO-d₆) δ 178.44, 38.49 (C×4), 36.04 (C×3), 30.71 (C×2), 27.38; GC-MS m/z: 180.25.

Malonic acid:¹²

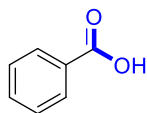


2m

Yield 82%; ¹H NMR (600.17 MHz, DMSO-d₆): δ 12.60 (br s, 2H), 3.23 (s, 2H); ¹³C NMR (150.92 MHz, DMSO-d₆) δ 168.50 (C×2), 41.99; GC-MS m/z: 104.05.

Note: Amides **1n-1r** generate acetic acid **2a** as the corresponding hydrolyzed product shown in Scheme 2.

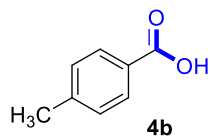
Benzoic acid:¹¹



4a

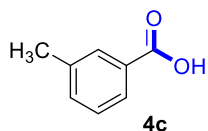
Yield 87%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 12.96 (s, 1H), 7.94 (d, J =8.04 Hz, 2H), 7.61 (t, J =6.87 Hz, 2H), 7.49 (t, J =6.87 Hz, 2H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 167.50, 133.02, 130.93, 129.44 (C \times 2), 128.73 (C \times 2); GC-MS m/z : 122.10.

4-Methylbenzoic acid:¹²



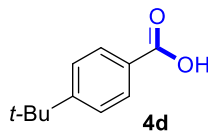
Yield 80%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 12.79 (s, 1H), 7.83 (d, J =7.68 Hz, 2H), 7.26 (d, J =7.68 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 167.41, 143.08, 129.41, 129.17, 128.12 (C \times 2), 21.17; GC-MS m/z : 136.15.

3-Methylbenzoic acid:⁵



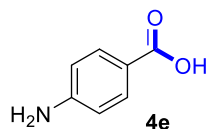
Yield 76%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 10.83 (s, 1H), 8.28 (d, J =8.22 Hz, 2H), 7.94 (d, J =8.14 Hz, 2H), 1.73 (s, 9H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 167.42, 137.90, 133.46, 130.74, 129.74, 128.46, 126.46, 20.82; GC-MS m/z : 136.15.

4-*tert*-Butylbenzoic acid:¹³



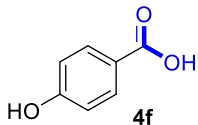
Yield 77%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 12.87 (s, 1H), 7.761 (d, J =8.10 Hz, 2H), 6.53 (d, J =8.10 Hz, 2H), 5.86 (br s, 2H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 166.27, 155.21, 130.37 (C \times 2), 127.83, 125.82 (C \times 2), 35.23, 31.44 (C \times 3); GC-MS m/z : 178.25.

4-Aminobenzoic acid:¹⁴



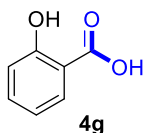
Yield 81%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 11.96 (br s, 1H), 7.79-7.71 (m, 2H), 7.42 (d, J =7.32 Hz, 1H), 7.39-7.34 (m, 1H), 2.35 (s, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 166.59, 153.21, 131.31(C \times 2), 116.93, 112.63 (C \times 2); GC-MS m/z : 137.15.

4-Hydroxybenzoic acid:¹⁵



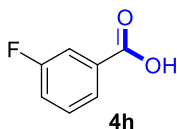
Yield 83%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 12.48 (br s, 1H), 10.27 (br s, 1H), 7.83 (d, J = 8.28 Hz, 2H), 6.85 (d, J = 8.28 Hz, 2H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 168.17, 162.58, 132.53, 122.32, 116.10; GC-MS m/z : 137.10.

2-Hydroxybenzoic acid:¹⁵



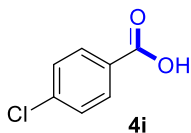
Yield 81%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 14.00 (br s, 1H), 11.30 (br s, 1H), 7.78 (d, J = 6.85 Hz, 1H), 7.52-7.48 (m, 1H), 6.96-7.91 (m, 2H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 171.95, 161.14, 135.69, 130.28, 119.21, 117.11, 112.66; GC-MS m/z : 137.10.

3-Fluorobenzoic acid:¹⁶



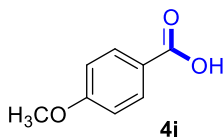
Yield 80%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 13.29 (br s, 1H), 7.77 (d, J = 7.08 Hz, 1H), 7.64 (d, J = 8.22 Hz, 1H), 7.57-7.51 (m, 1H), 7.46 (t, J = 7.56 Hz, 1H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 166.25, 162.02 (d, J = 244.20 Hz), 133.30 (d, J = 6.03 Hz), 130.82 (d, J = 6.03 Hz), 125.48, 119.89 (d, J = 20.23 Hz), 115.79 (d, J = 22.63 Hz); GC-MS m/z : 140.10.

4-Fluorobenzoic acid:¹⁶



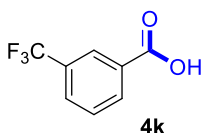
Yield 84%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 13.17 (br s, 1H), 7.92 (d, J = 8.07 Hz, 2H), 7.52 (d, J = 8.07 Hz, 2H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 166.53, 137.87, 131.19, 129.69, 128.77 (C \times 2); GC-MS m/z : 156.55.

4-Methoxybenzoic acid:¹²



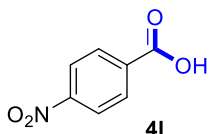
Yield 83%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 12.62 (s, 1H), 7.85 (d, J = 8.75 Hz, 2H), 7.00 (d, J = 8.75 Hz, 2H), 3.82 (s, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 167.01, 162.85, 131.36 (C \times 2), 122.83, 113.82 (C \times 2), 55.45; GC-MS m/z : 152.15.

3-(Trifluoromethyl)benzoic acid:¹⁷



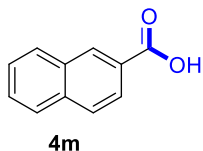
Yield 84%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 13.54 (s, 1H), 8.21 (d, $J=7.02$ Hz, 1H), 8.16 (s, 1H), 7.97 (d, $J=8.10$ Hz, 1H), 7.74 (d, $J=7.56$ Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 166.06, 133.23, 132.04, 130.07, 129.46(d, $J=24.14$ Hz), 129.35 (d, $J=4.33$ Hz), 125.54 (d, $J=4.33$ Hz), 123.83 (d, $J=271.65$ Hz); GC-MS m/z: 190.10

4-Nitrobenzoic acid:⁵



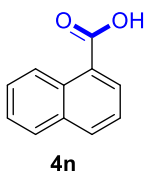
Yield 76%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 13.66 (s, 1H), 8.30 (d, $J=7.98$ Hz, 1H), 8.15 (d, $J=7.98$ Hz, 1H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 166.83, 150.05, 136.38, 130.72 (C \times 2), 123.74 (C \times 2); GC-MS m/z: 167.10.

Naphthalen-2-carboxylic acid:¹⁶



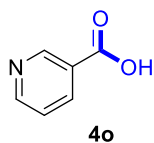
Yield 86%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 13.10 (br s, 1H), 8.61 (s, 1H), 8.10 (d, $J=7.98$ Hz, 1H), 8.01-7.94 (m, 3 H), 7.64 (t, $J=7.44$ Hz, 1H), 7.59 (d, $J=7.44$ Hz, 1H), 7.57 (t, $J=7.56$ Hz, 1H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 167.49, 134.96, 132.18, 130.56, 129.31, 128.35, 128.20, 128.10 (C \times 2), 127.68 (C \times 2), 126.84, 125.20; GC-MS m/z: 172.15.

Naphthalen-1-carboxylic acid:¹¹



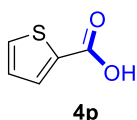
Yield 82%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 13.15 (br s, 1H), 8.85 (d, $J=7.98$ Hz, 1H), 8.14 (d, $J=6.90$ Hz, 2H), 8.01 (d, $J=6.84$ Hz, 1H), 7.63 (t, $J=7.22$ Hz, 1H), 7.58 (d, $J=7.82$ Hz, 2H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 168.66, 133.47, 132.95, 130.68, 129.87, 128.62, 127.52, 126.20, 124.89; GC-MS m/z: 172.15.

Nicotinic acid:¹⁶



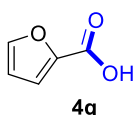
Yield 83%; ^1H NMR (600.17 MHz, DMSO- d_6): δ 13.43 (br s, 1H), 8.77 (d, $J=7.56$ Hz, 1H), 8.25 (d, $J=8.04$ Hz, 1H), 7.52 (t, $J=8.04$ Hz, 1H); ^{13}C NMR (150.92 MHz, DMSO- d_6) δ 166.34, 153.32, 150.29, 137.02, 126.63, 123.85; GC-MS m/z: 123.10.

Thiophene-2-carboxylic acid:¹⁸



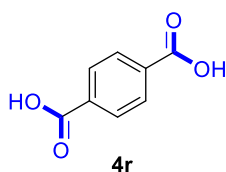
Yield 85%; ¹H NMR (600.17 MHz, DMSO-d₆): δ 13.04 (br s, 1H), 7.90-7.86 (m, 1H), 7.72 (d, *J* = 7.02 Hz, 1H), 7.18 (t, *J* = 6.54 Hz, 1H); ¹³C NMR (150.92 MHz, DMSO-d₆) δ 162.94, 134.67, 133.30, 133.25, 128.25; GC-MS *m/z*: 128.15.

Furan-2-carboxylic acid:¹⁹



Yield 85%; ¹H NMR (600.17 MHz, DMSO-d₆): δ 13.08 (br s, 1H), 7.94 (s, 1H), 7.24 (d, *J* = 4.14 Hz, 1H), 6.68-6.67 (m, 1H); ¹³C NMR (150.92 MHz, DMSO-d₆) δ 160.32, 148.05, 145.88, 118.72, 113.10; GC-MS *m/z*: 112.10.

Terephthalic acid:²⁰



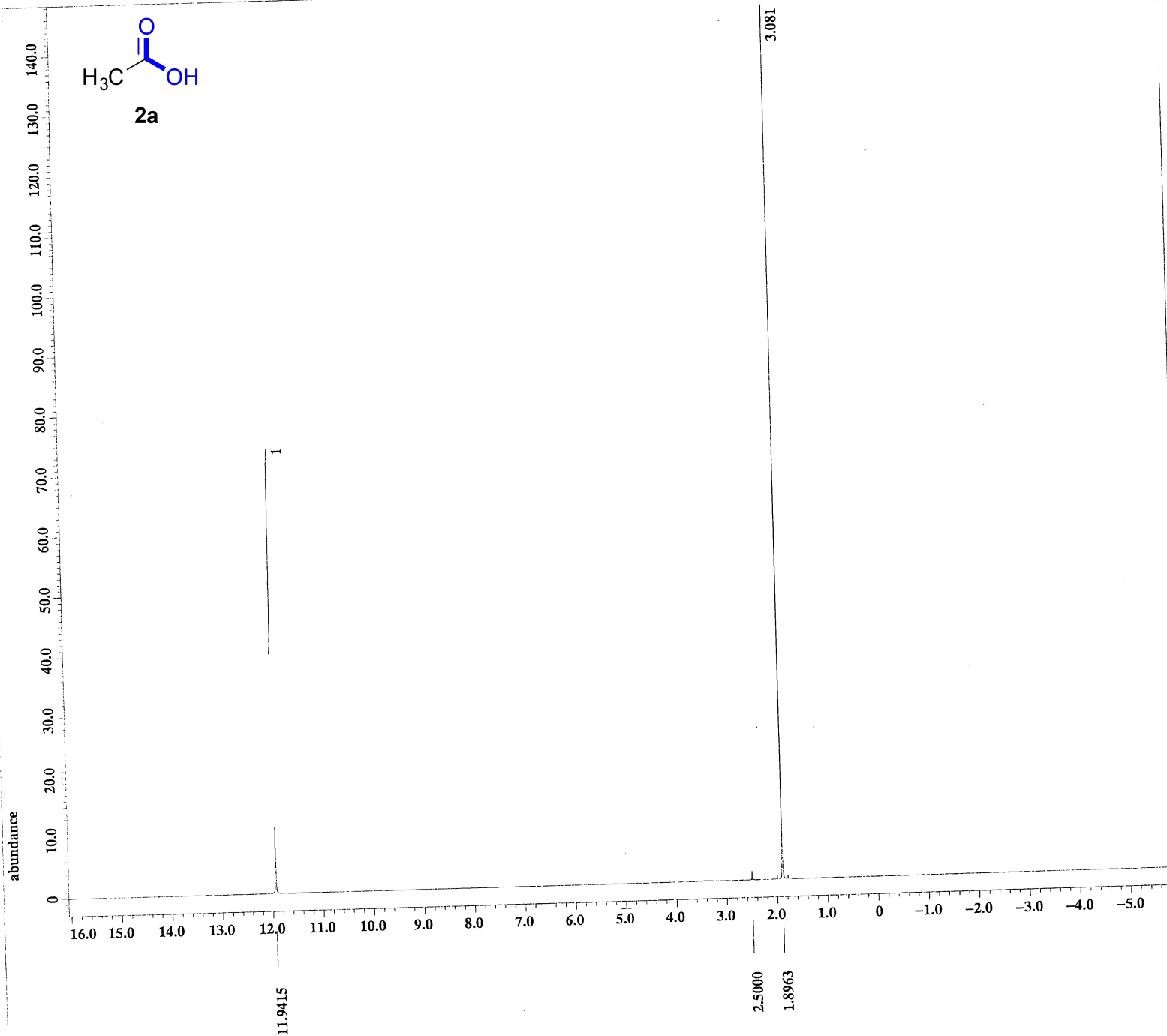
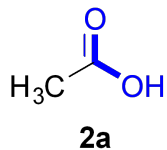
Yield 83%; ¹H NMR (600.17 MHz, DMSO-d₆): δ 13.29 (br s, 2H), 8.05 (s, 4H); ¹³C NMR (150.92 MHz, DMSO-d₆) δ 166.74 (C×2), 134.50 (C×2), 129.53 (C×4); GC-MS *m/z*: 166.15.

Note: Amides **3s-3w** generate benzoic acid **4a** as the corresponding hydrolyzed product shown in section (B) of Scheme 4.

REFERENCES

- 1 M. Tamura, K. Shimizu and A. Satsuma, *Applied Catal. A, Gen.*, 2012, **433-434**, 135-145.
- 2 Q. J. Yan, S. Q. Yang, X. J. Duan, H. B. Xu, Y. Liu and Z. Q. Jiang, *J. Mol. Catal. B Enzym.*, 2014, **109**, 76-84.
- 3 Y. Hirai, T. Kojima, Y. Mizutani, Y. Shiota, K. Yoshizawa and S. Fukuzumi, *Angew. Chemie*, 2008, **120**, 5856-5860.
- 4 H. Tsunoyama, T. Tsukuda and H. Sakurai, *Chem. Lett.*, 2007, **36**, 212-213.
- 5 A. T. Murray, P. Matton, N. W. G. Fairhurst, M. P. John and D. R. Carbery, *Org. Lett.*, 2012, **14**, 3656-3659.
- 6 O. Itsenko and B. Långström, *J. Org. Chem.*, 2005, **70**, 2244-2249.
- 7 J. C. Lee, E. S. Yoo and J. S. Lee, *Synth. Commun.*, 2004, **34**, 3017-3020.
- 8 T. Osako, R. Kaiser, K. Torii and Y. Uozumi, *Synlett*, 2019, **30**, 961-966.
- 9 S. M. A. H. Siddiki, A. S. Touchy, K. Kon, T. Toyao and K. Shimizu, *ChemCatChem*, 2017, **9**, 2816-2821.
- 10 C. J. Salomon, E. G. Mata and O. A. Mascaretti, *J. Org. Chem.*, 1994, **59**, 7259-7266.
- 11 V. Cherepakhin and T. J. Williams, *ACS Catal.*, 2018, **8**, 3754-3763.

- 12 S. M. A. H. Siddiki, T. Toyao, K. Kon, A. S. Touchy and K. Shimizu, *J. Catal.*, 2016, **344**, 741–748.
- 13 K. Lee, Y. H. Kim, S. B. Han, H. Kang, S. Park, W. S. Seo, J. T. Park, B. Kim and S. Chang, *J. Am. Chem. Soc.*, 2003, **125**, 6844–6845.
- 14 C. Wiles, P. Watts and S. J. Haswell, *Tetrahedron Lett.*, 2006, **47**, 5261–5264.
- 15 D. Sang, C. Yi, Z. He, J. Wang, J. Tian, M. Yao and H. Shi, *Tetrahedron Lett.*, 2018, **59**, 1469–1472.
- 16 H. M. Liu, L. Jian, C. Li, C. C. Zhang, H. Y. Fu, X. L. Zheng, H. Chen and R. X. Li, *J. Org. Chem.*, 2019, **84**, 9151–9160.
- 17 N. Iqbal, S. Choi, Y. You and E. J. Cho, *Tetrahedron Lett.*, 2013, **54**, 6222–6225.
- 18 L. Han, P. Xing and B. Jiang, *Org. Lett.*, 2014, **16**, 3428–3431.
- 19 P. Sathyanarayana, A. Upare, O. Ravi, P. R. Muktapuram and S. R. Bathula, *RSC Adv.*, 2016, **6**, 22749–22753.
- 20 T. Nakai, T. Iwai, M. Mihara, T. Ito and T. Mizuno, *Tetrahedron Lett.*, 2010, **51**, 2225–2227.



```

Filename      = Exp-R-124-27a-P-3.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-27a-P
Solvent      = DMSO-D6
Creation_time = 29-AUG-2018 19:16:17
Revision_time = 29-AUG-2018 19:21:04
Current_time = 29-AUG-2018 19:21:08
  
```

```

Content      = Exp-R-124-27a-P
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR
  
```

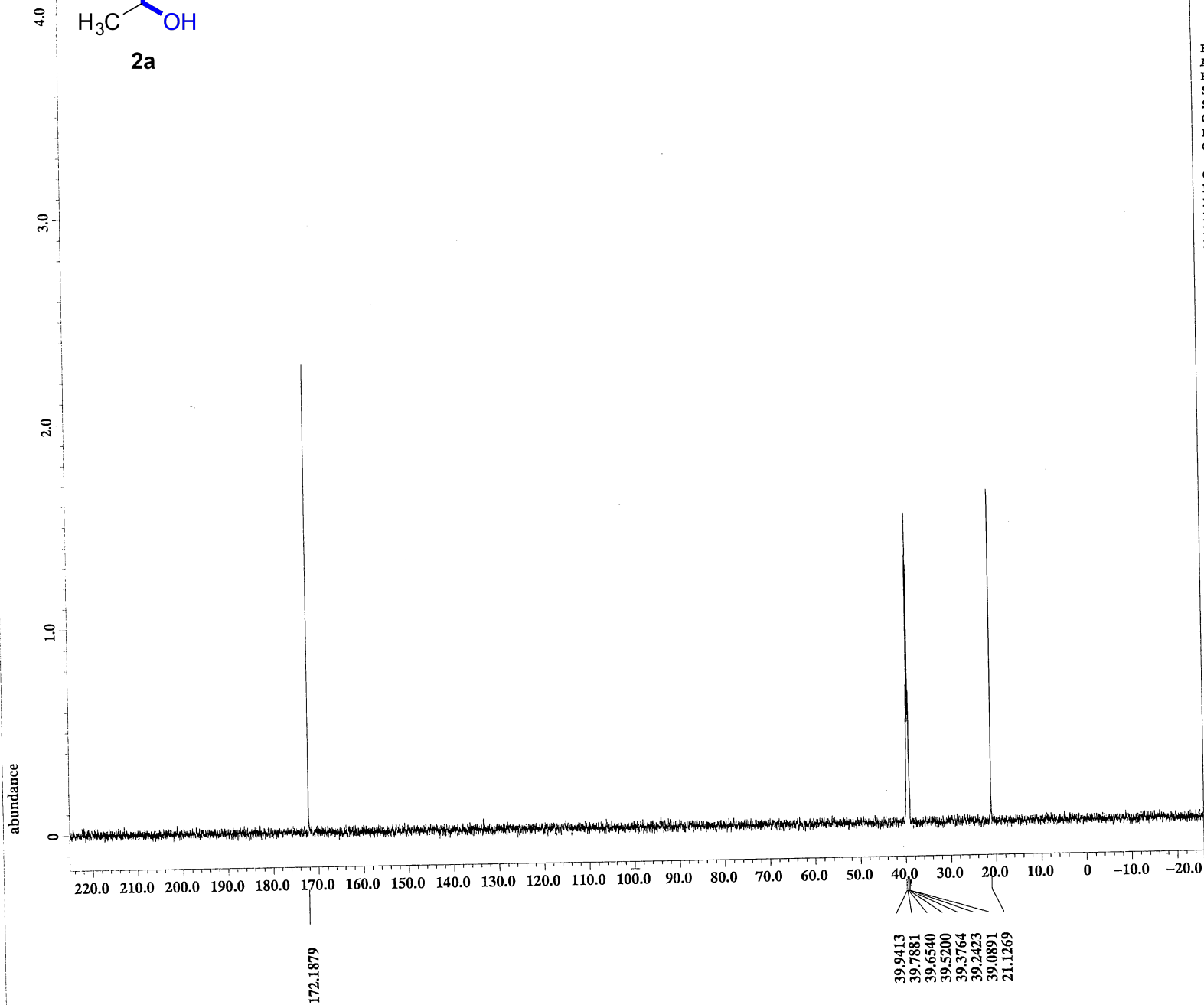
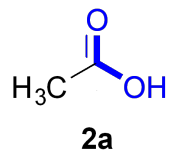
```

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 1.00917917[Hz]
X_sweep        = 16.53439153[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8
  
```

```

X_90_width    = 12.68[us]
X_acq_time     = 0.99090432[s]
X_angle        = 45[deg]
X_atn          = 3.4[dB]
X_pulse        = 6.34[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 40
Relaxation_delay = 5[s]
Repetition_time = 5.99090432[s]
Temp_get       = 21.3[dC]
  
```

X : parts per Million : 1H



X : parts per Million : 13C

```

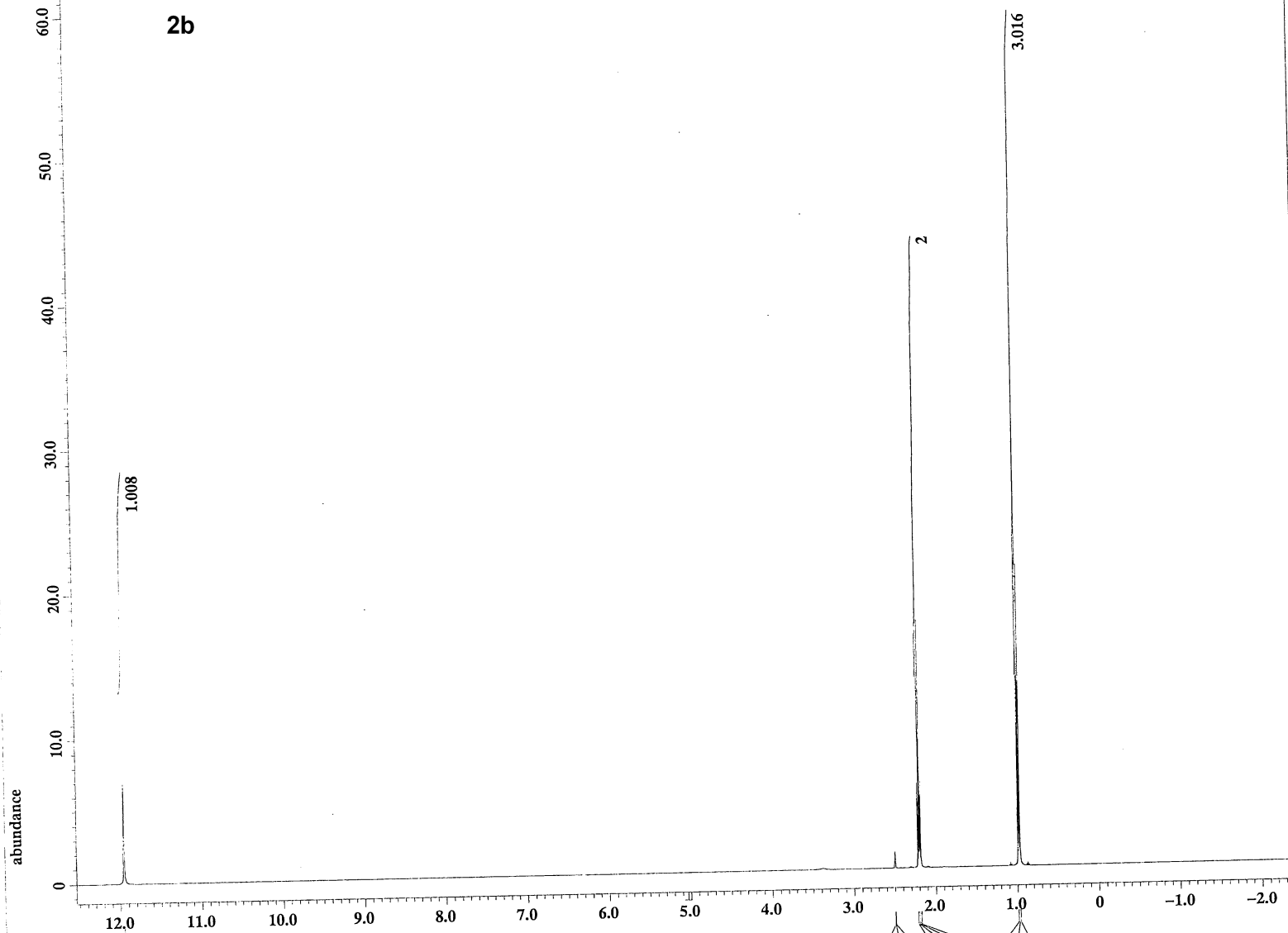
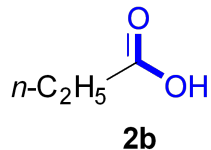
Filename      = Exp-R-124-27a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-27a-C
Solvent      = DMSO-D6
Creation_time = 29-AUG-2018 19:19:40
Revision_time = 29-AUG-2018 19:21:51
Current_time  = 29-AUG-2018 19:22:01

Content      = Exp-R-124-27a-C
Data_format  = 1D_COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 48
Total_scans    = 48

X_90_width     = 12[us]
X_acq_time     = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 7.5[dB]
X_pulse        = 4[us]
Irr_atn_dec    = 18.95[dB]
Irr_atn_noe    = 18.95[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2.5[s]
Recvr_gain     = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get       = 21.8[dC]

```



```

Filename      = Exp-R-124-3a-P-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-3a-P
Solvent      = DMSO-D6
Creation_time = 3-SEP-2018 17:04:25
Revision_time = 3-SEP-2018 17:09:34
Current_time  = 3-SEP-2018 17:09:37
  
```

```

Content      = Exp-R-124-3a-P
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR
  
```

```

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 1.4548992[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.68733284[Hz]
X_sweep        = 11.26126126[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8
  
```

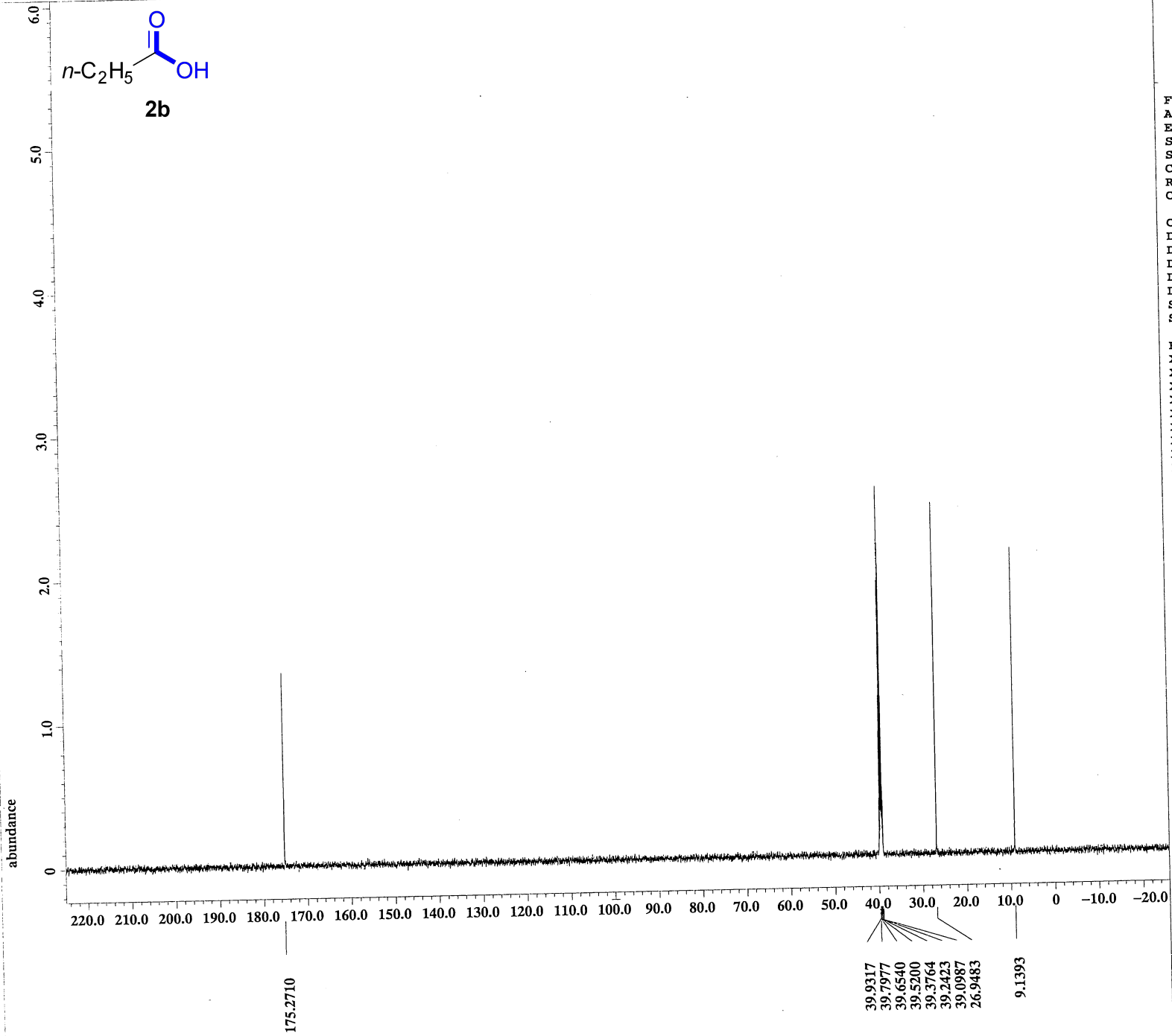
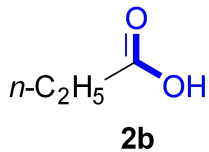
```

X_90_width    = 12.68[us]
X_acq_time     = 1.4548992[s]
X_angle        = 45[deg]
X_atn          = 3.4[dB]
X_pulse        = 6.34[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 40
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get       = 21.5[dC]
  
```

11.9584

2.5023
 2.5000
 2.4966
 2.2206
 2.2080
 2.1954
 2.1839
 0.9929
 0.9803
 0.9677

X : parts per Million : 1H



```

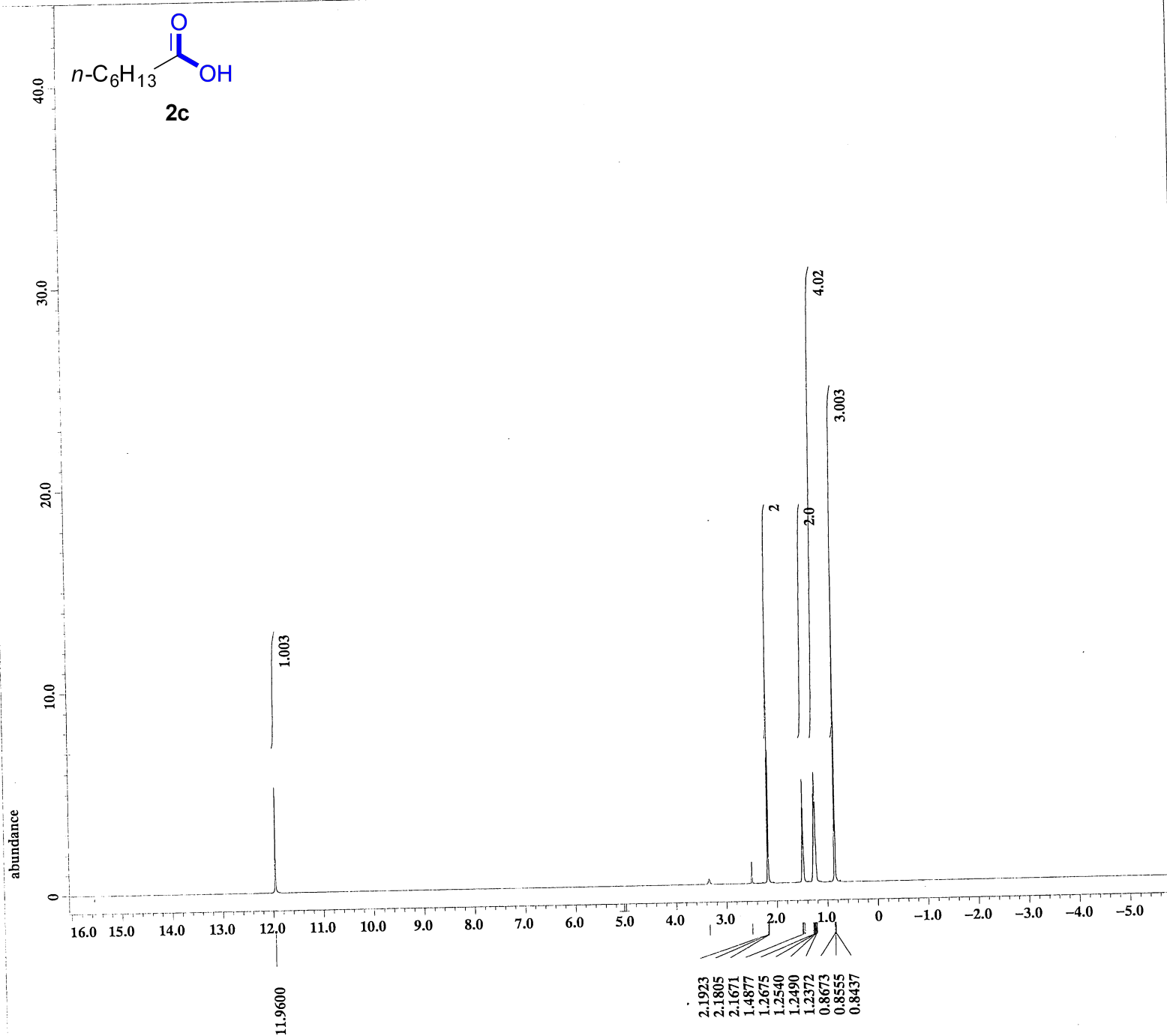
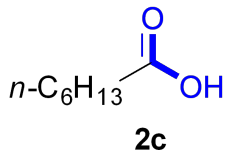
Filename      = Exp-R-124-3a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-3a-C
Solvent      = DMSO-D6
Creation_time = 3-SEP-2018 17:07:38
Revision_time = 3-SEP-2018 17:10:14
Current_time  = 3-SEP-2018 17:10:25

Content      = Exp-R-124-3a-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 45
Total_scans    = 45

X_90_width    = 12[us]
X_acq_time     = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 7.5[dB]
X_pulse        = 4[us]
Irr_atn_dec    = 18.95[dB]
Irr_atn_noe    = 18.95[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2.5[s]
Recvr_gain     = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get       = 22.2[dc]
  
```

X : parts per Million : 13C



```

Filename      = Exp-R-124-10a-P-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-10a-P
Solvent      = DMSO-D6
Creation_time = 3-SEP-2018 17:15:21
Revision_time = 3-SEP-2018 17:20:28
Current_time  = 3-SEP-2018 17:20:31

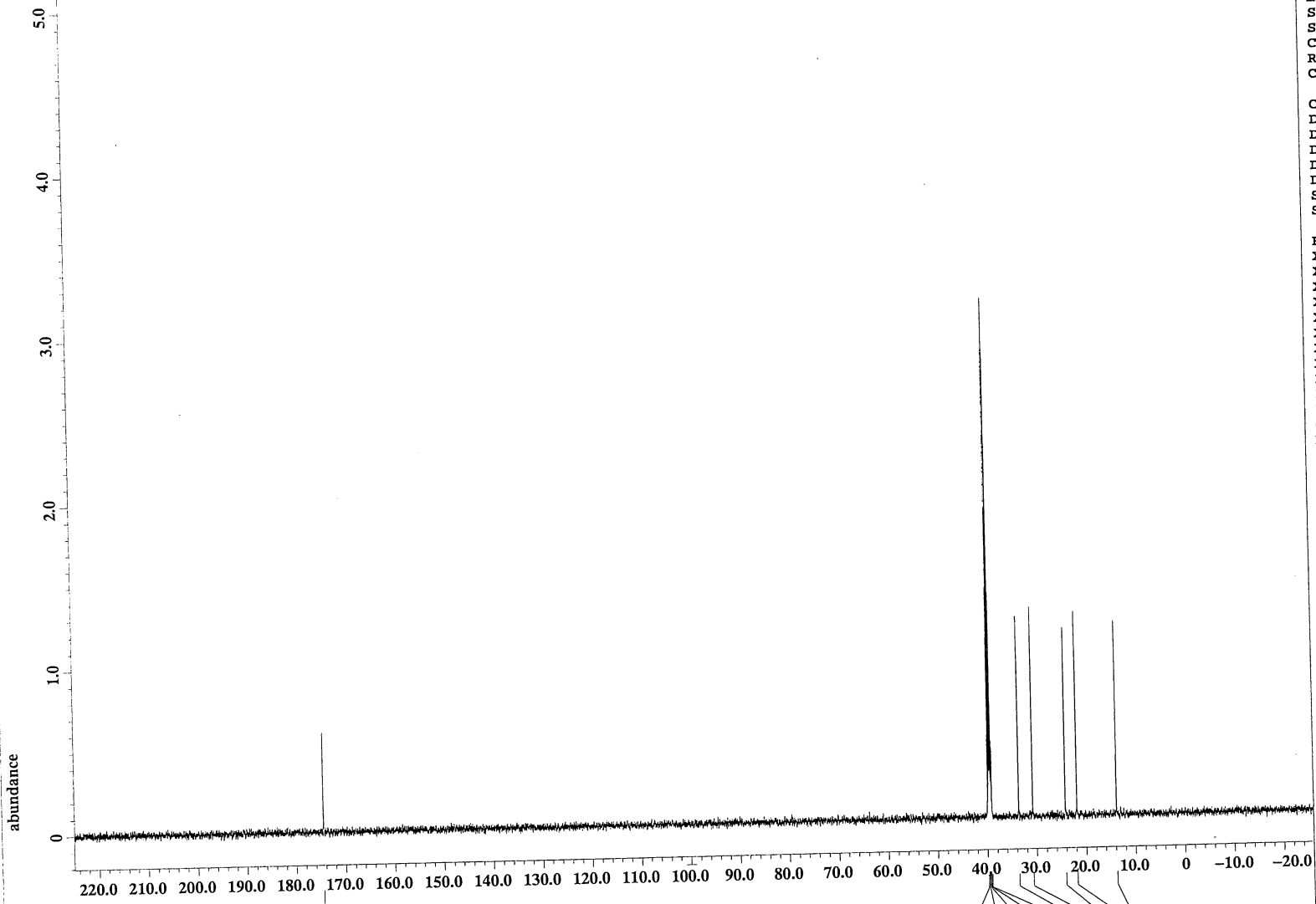
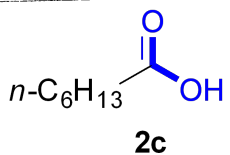
Content      = Exp-R-124-10a-P
Data_format  = 1D_COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain       = 1H
X_freq        = 600.1723046[MHz]
X_offset      = 5[ppm]
X_points      = 16384
X_prescans    = 1
X_resolution  = 1.00917917[Hz]
X_sweep       = 16.53439153[kHz]
Irr_domain    = 1H
Irr_freq      = 600.1723046[MHz]
Irr_offset    = 5[ppm]
Tri_domain    = 1H
Tri_freq      = 600.1723046[MHz]
Tri_offset    = 5[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 8
Total_scans   = 8

X_90_width   = 12.68[us]
X_acq_time    = 0.99090432[s]
X_angle       = 45[deg]
X_atn        = 3.4[dB]
X_pulse      = 6.34[us]
Irr_mode     = Off
Tri_mode     = Off
Dante_presat = FALSE
Initial_wait  = 1[s]
Recvr_gain   = 40
Relaxation_delay = 5[s]
Repetition_time = 5.99090432[s]
Temp_get     = 21.9[dc]

```

X : parts per Million : 1H



```

Filename      = Exp-R-124-10a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-10a-C
Solvent      = DMSO-D6
Creation_time = 3-SEP-2018 17:18:33
Revision_time = 3-SEP-2018 17:21:00
Current_time  = 3-SEP-2018 17:21:23

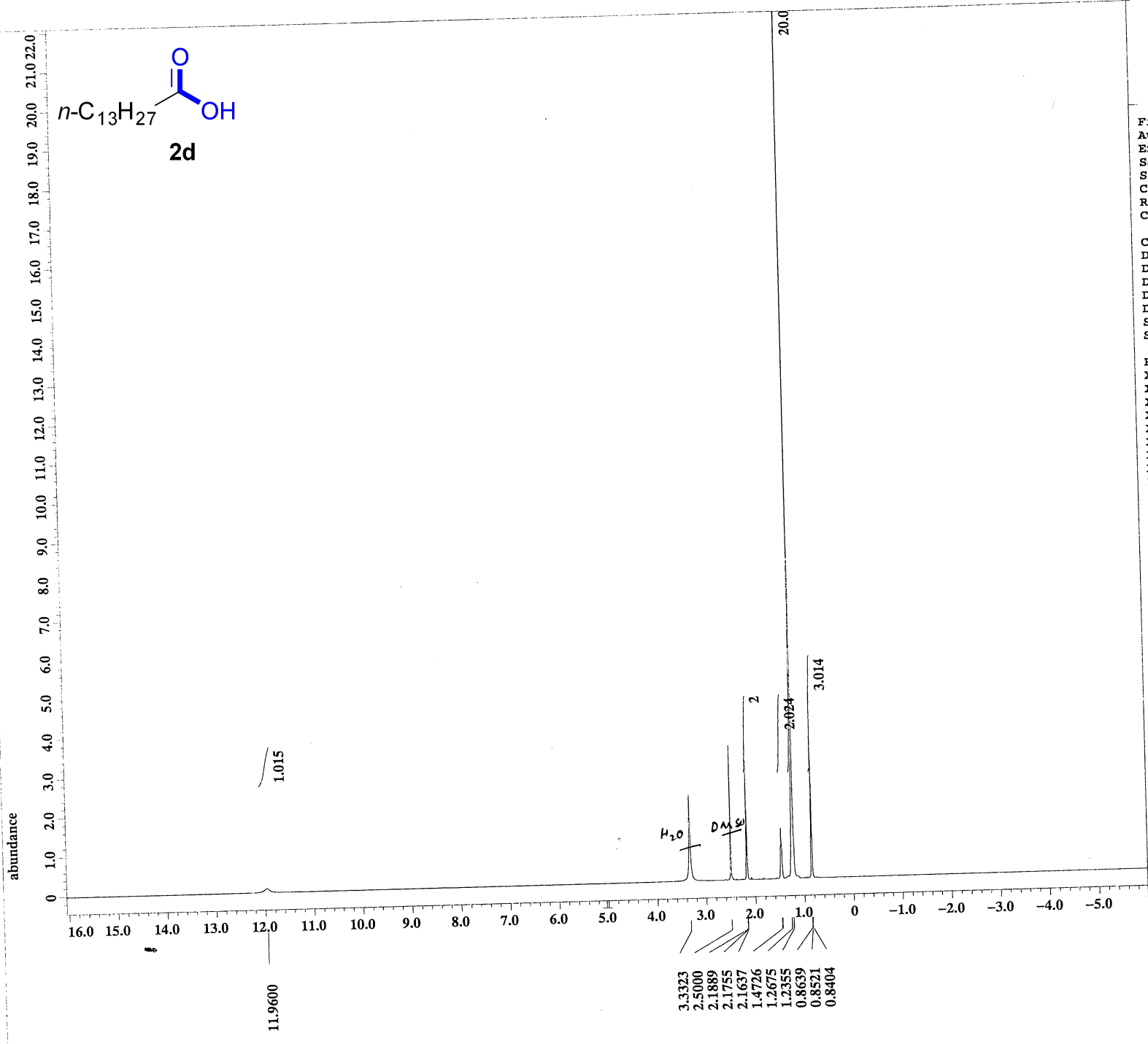
Content      = Exp-R-124-10a-C
Data_format  = 1D_COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 45
Total_scans    = 45

X_90_width    = 12[us]
X_acq_time    = 0.69206016[s]
X_angle       = 30[deg]
X_atn         = 7.5[dB]
X_pulse       = 4[us]
Irr_atn_dec   = 18.95[dB]
Irr_atn_noe   = 18.95[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 2.5[s]
Recvr_gain    = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get      = 22.4[dc]

```

X : parts per Million : 13C



```

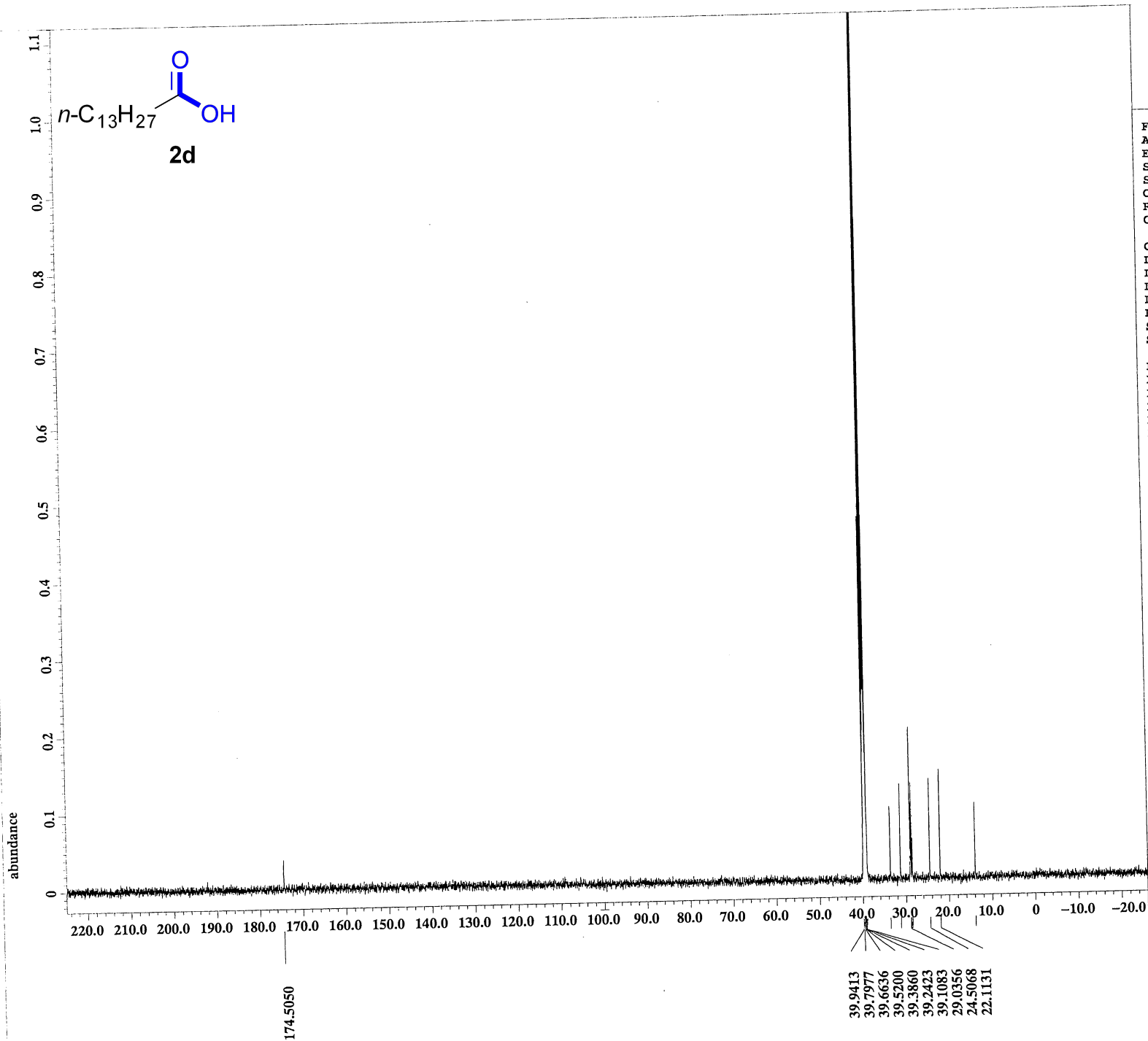
Filename      = Exp-R-122-5a-P-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-122-5a-P
Solvent      = DMSO-D6
Creation_time = 1-AUG-2018 18:53:36
Revision_time = 1-AUG-2018 19:26:56
Current_time  = 1-AUG-2018 19:27:00

Content      = Exp-R-122-5a-P
Data_format  = 1D_COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA_600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans    = 1
X_resolution   = 1.00917917[Hz]
X_sweep        = 16.53439153[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 12.68[us]
X_acq_time     = 0.99090432[s]
X_angle        = 45[deg]
X_atn          = 3.4[dB]
X_atn         = 6.34[us]
X_pulse        = Off
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 48
Relaxation_delay = 5[s]
Repetition_time = 5.99090432[s]
Temp_get       = 21.8[dc]
  
```

X : parts per Million : 1H



```

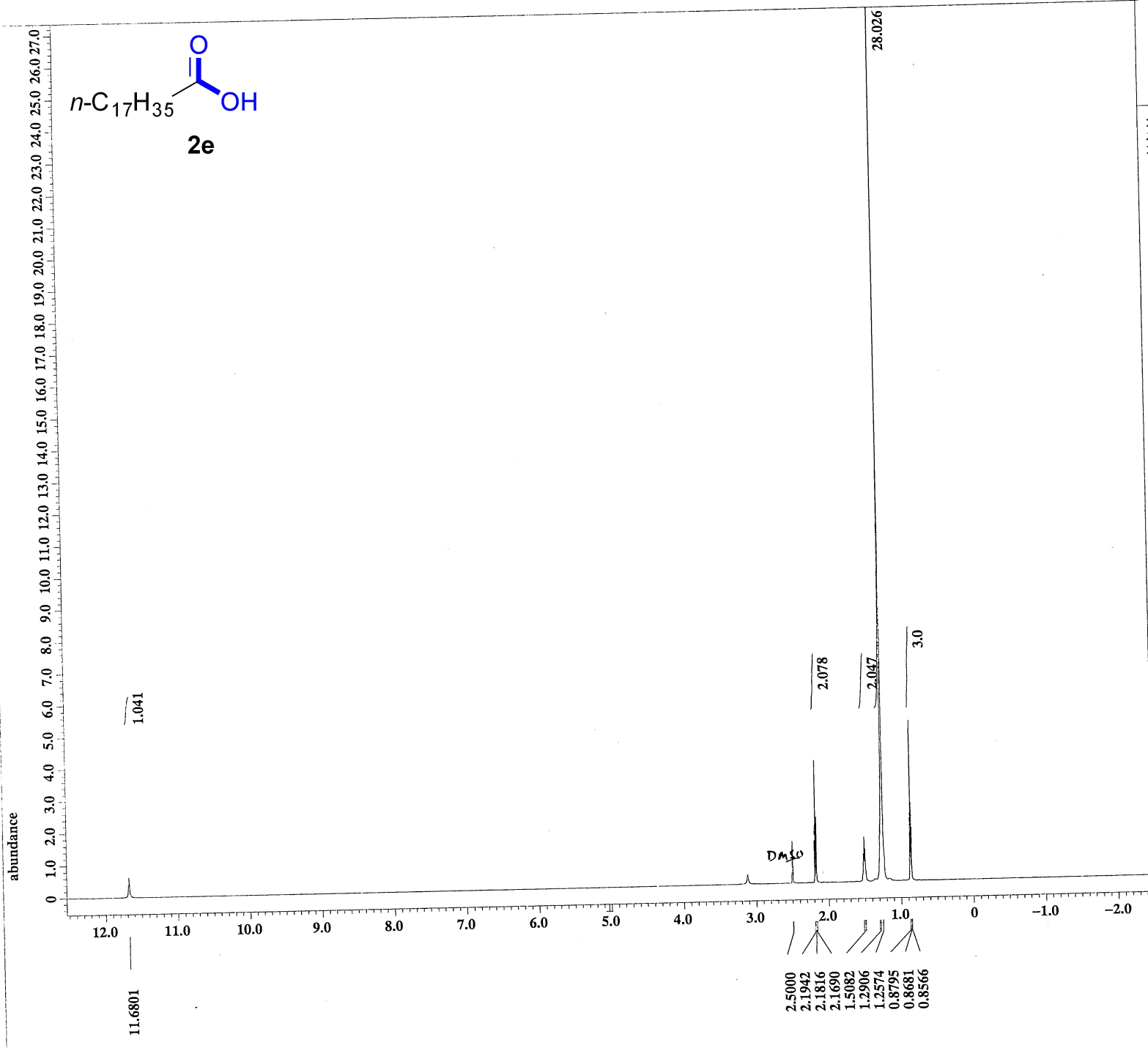
Filename      = Exp-R-122-5a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-122-5a-C
Solvent      = DMSO-D6
Creation_time = 1-AUG-2018 19:37:16
Revision_time = 1-AUG-2018 20:07:53
Current_time  = 1-AUG-2018 20:08:23

Content      = Exp-R-122-5a-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = TRUE
Mod_return     = 1
Scans          = 805
Total_scans    = 805

X_90_width    = 12[us]
X_acq_time    = 0.69206016[s]
X_angle       = 30[deg]
X_atn         = 7.5[dB]
X_pulse       = 4[us]
Irr_atn_dec   = 18.95[dB]
Irr_atn_noe   = 18.95[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 2.5[s]
Recvr_gain    = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get      = 22.5[dc]
  
```

X : parts per Million : 13C



```

Filename      = Exp-R-124-9a-proton-4
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-9a-proton
Solvent      = DMSO-D6
Creation_time = 20-SEP-2018 12:27:22
Revision_time = 20-SEP-2018 12:37:22
Current_time  = 20-SEP-2018 12:37:26

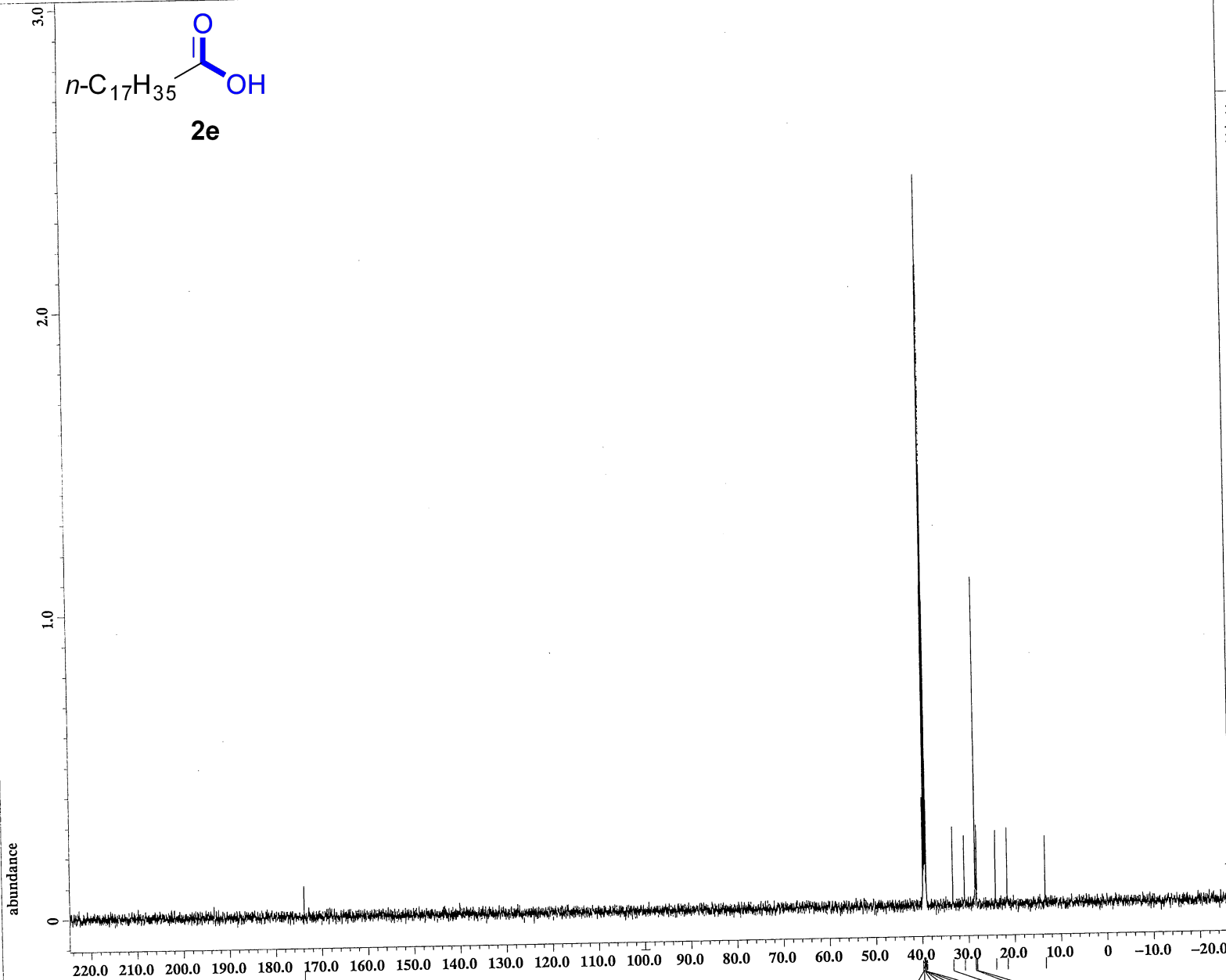
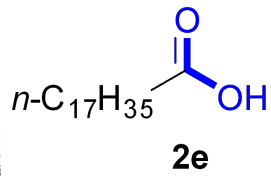
Content      = Exp-R-124-9a-proton
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 1.4548992[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.68733284[Hz]
X_sweep        = 11.26126126[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 12.68[us]
X_acq_time     = 1.4548992[s]
X_angle        = 45[deg]
X_atn          = 3.4[dB]
X_pulse        = 6.34[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 44
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get       = 70[dc]

```

X : parts per Million : 1H



Filename = Exp-R-124-9a-Carbon-4
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = Exp-R-124-9a-Carbon
 Solvent = DMSO-D6
 Creation_time = 20-SEP-2018 12:32:40
 Revision_time = 20-SEP-2018 12:38:58
 Current_time = 20-SEP-2018 12:39:50

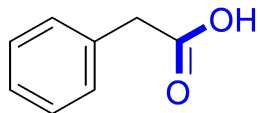
Content = Exp-R-124-9a-Carbon
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.69206016[s]
 X_domain = 13C
 X_freq = 150.91343039 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109 [Hz]
 X_sweep = 47.34848485 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 102
 Total_scans = 102

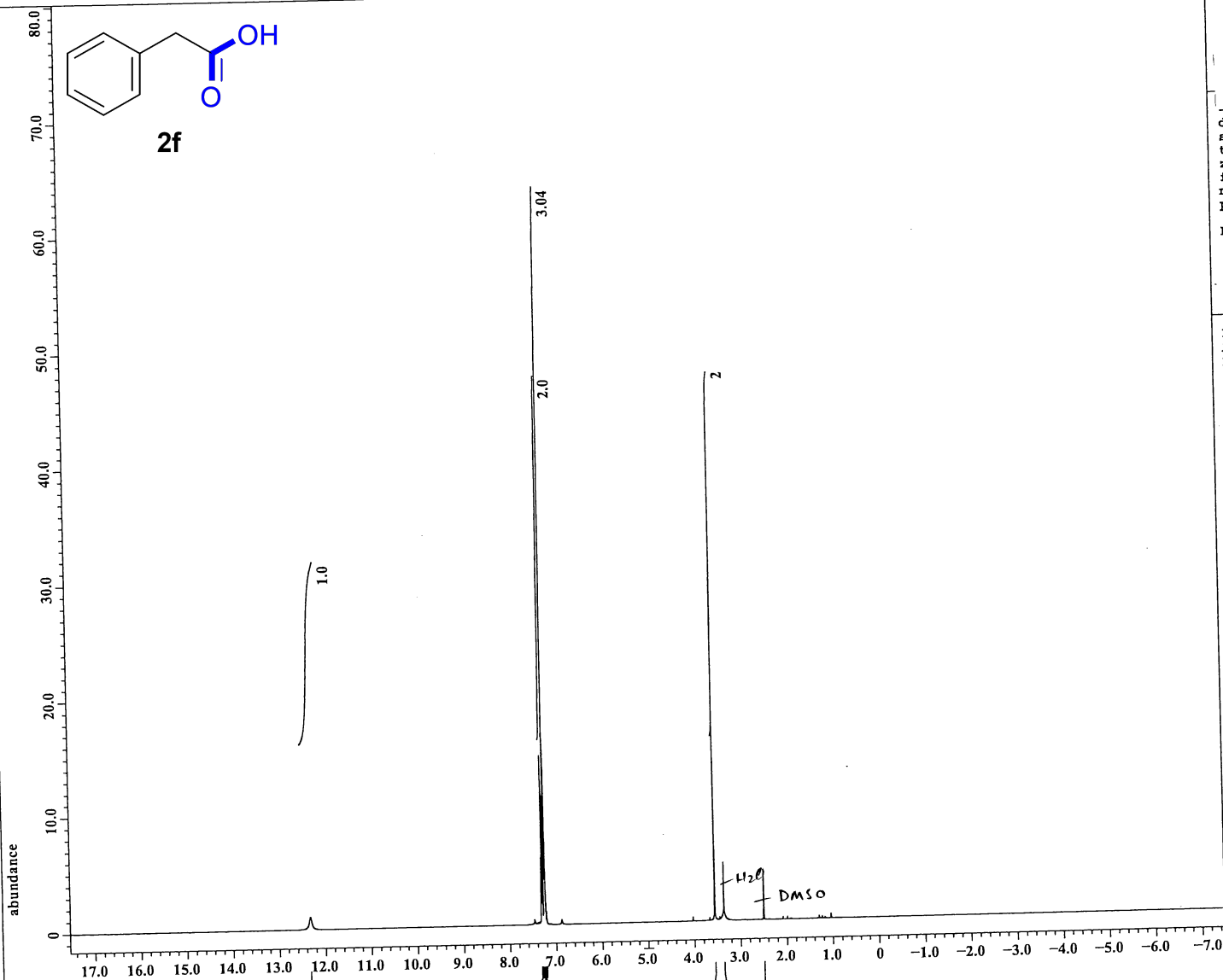
X_90_width = 12 [us]
 X_acq_time = 0.69206016 [s]
 X_angle = 30 [deg]
 X_atn = 7.5 [dB]
 X_pulse = 4 [us]
 Irr_atn_dec = 18.95 [dB]
 Irr_atn_noe = 18.95 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.69206016 [s]
 Temp_get = 70 [dC]

- 39.9317
- 39.7977
- 39.6540
- 39.5200
- 39.3764
- 39.2423
- 39.0987
- 33.4017
- 28.6143
- 28.2697

X : parts per Million : 13C



2f



X : parts per Million : 1H

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

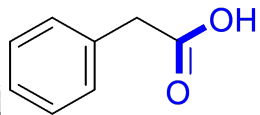
Derived from: Exp-R-163-6-1a-P-1.jdf

Filename = Exp-R-163-6-1a-P-4.jd
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-163-6-1a-P
 Solvent = DMSO-D6
 Creation_time = 18-DEC-2018 12:19:52
 Revision_time = 18-DEC-2018 12:24:20
 Current_time = 18-DEC-2018 12:24:50

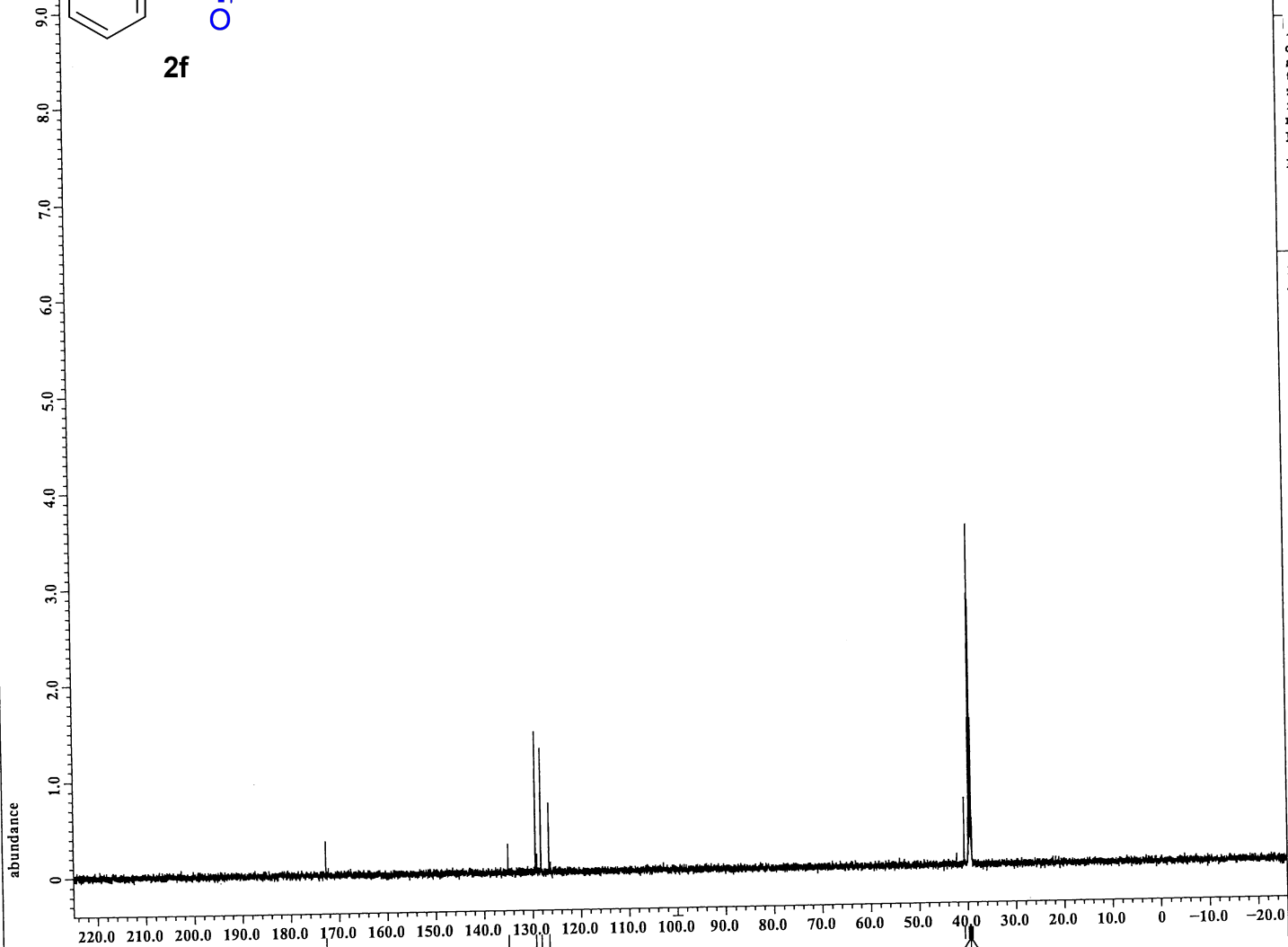
Comment = Exp-R-163-6-1a-P
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.87293952[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.14555473[Hz]
 X_sweep = 18.76876877[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17[us]
 X_acq_time = 0.87293952[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.585[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 5[s]
 Repetition_time = 5.87293952[s]
 Temp_get = 20.9[dc]



2f



X : parts per Million : 13C

----- 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

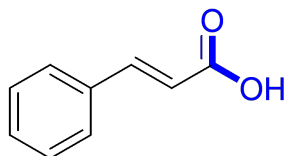
Derived from: Exp-R-163-6-1a-C-2.jdf

Filename = Exp-R-163-6-1a-C-4.jd
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = Exp-R-163-6-1a-C
 Solvent = DMSO-D6
 Creation_time = 18-DEC-2018 12:30:56
 Revision_time = 18-DEC-2018 12:33:40
 Current_time = 18-DEC-2018 12:34:16

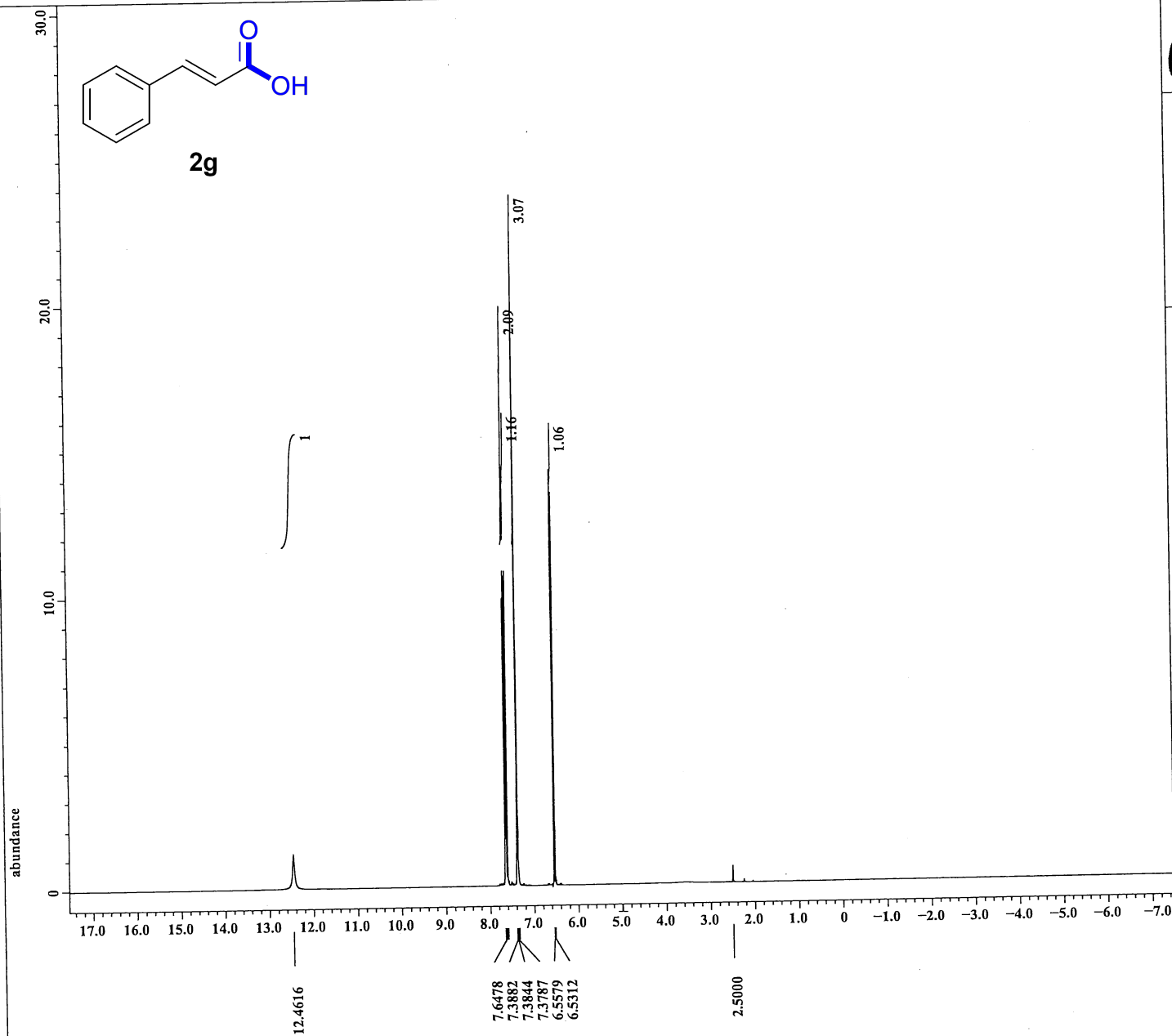
Comment = Exp-R-163-6-1a-C
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M])
 X_acq_duration = 0.69206016 [s]
 X_domain = 13C
 X_freq = 150.91343039 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109 [Hz]
 X_sweep = 47.34848485 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 21
 Total_scans = 21

X_90_width = 12.7 [us]
 X_acq_time = 0.69206016 [s]
 X_angle = 30 [deg]
 X_atn = 7.5 [dB]
 X_pulse = 4.23333333 [us]
 Irr_atn_dec = 18.62 [dB]
 Irr_atn_noe = 18.62 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.69206016 [s]
 Temp_get = 21.2 [dC]



2g



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

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

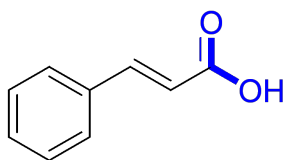
Derived from: Exp-R-124-8-1-P-1.jdf

Filename = Exp-R-124-8-1-P-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-124-8-1-P
 Solvent = DMSO-D6
 Creation_time = 12-DEC-2018 17:57:02
 Revision_time = 12-DEC-2018 18:07:36
 Current_time = 12-DEC-2018 18:08:43

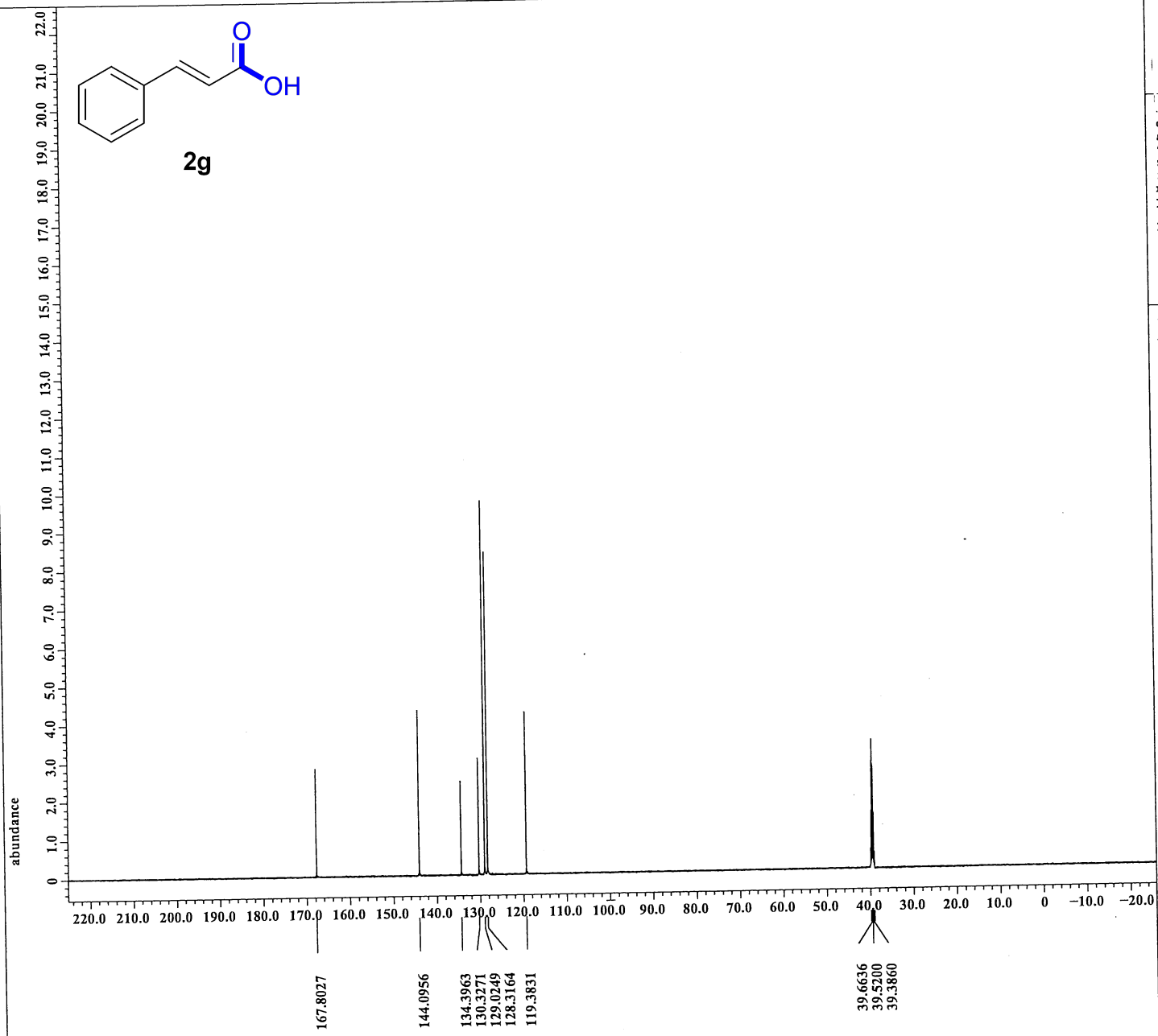
Comment = Exp-R-124-8-1-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M
 X_acq_duration = 0.87293952 [s]
 X_domain = 1H
 X_freq = 600.1723046 [MHz]
 X_offset = 5 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.14555473 [Hz]
 X_sweep = 18.76876877 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17 [us]
 X_acq_time = 0.87293952 [s]
 X_angle = 45 [deg]
 X_atn = 3.4 [dB]
 X_atn = 6.585 [us]
 X_pulse = Off
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 30
 Relaxation_delay = 5 [s]
 Repetition_time = 5.87293952 [s]
 Temp_get = 20.5 [dC]



2g



X : parts per Million : 13C

```

----- 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: Exp-R-124-8-1-C-1.jdf

```

Filename      = Exp-R-124-8-1-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-8-1-C
Solvent      = DMSO-D6
Creation time = 12-DEC-2018 18:03:00
Revision time = 12-DEC-2018 18:06:19
Current_time = 12-DEC-2018 18:07:20

```

```

Comment      = Exp-R-124-8-1-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

```

```

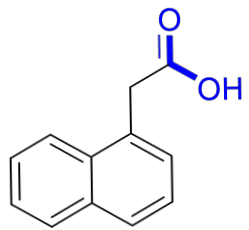
Field_strength = 14.09636928 [T] (600 [M])
X_acq_duration = 0.69206016 [s]
X_domain       = 13C
X_freq         = 150.91343039 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109 [Hz]
X_sweep        = 47.34848485 [kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046 [MHz]
Irr_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 117
Total_scans    = 117

```

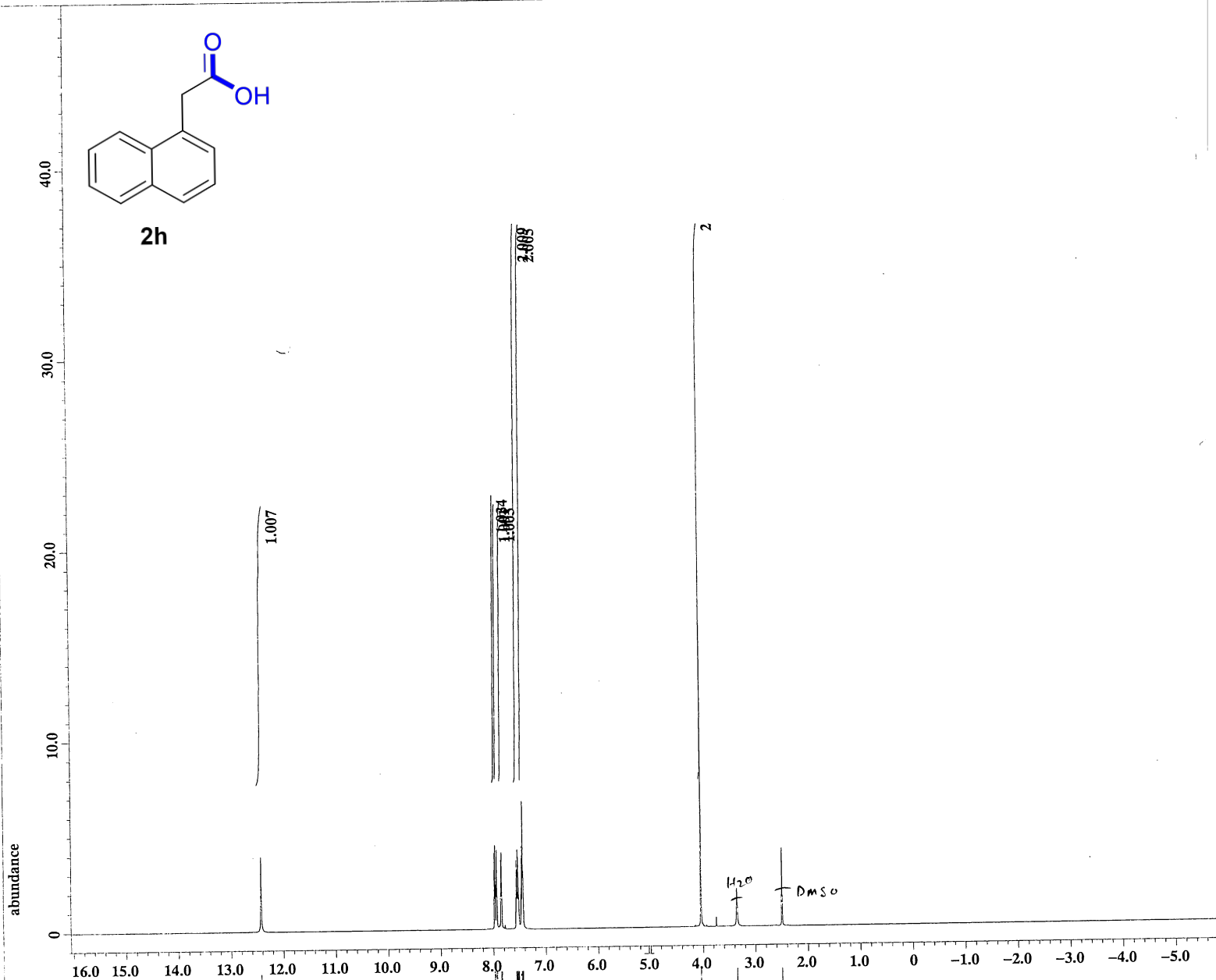
```

X_90_width    = 12.7 [us]
X_acq_time     = 0.69206016 [s]
X_angle        = 30 [deg]
X_atn          = 7.5 [dB]
X_pulse        = 4.23333333 [us]
Irr_atn_dec    = 18.62 [dB]
Irr_atn_noe    = 18.62 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.69206016 [s]
Temp_get       = 21.3 [dC]

```



2h



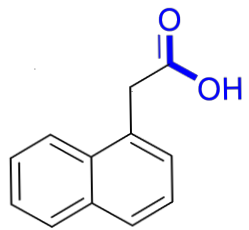
X : parts per Million : 1H

Sample_id = Exp-R-124-1-nap-aceti
 Solvent = DMSO-D6
 Creation_time = 21-SEP-2018 19:42:34
 Revision_time = 21-SEP-2018 19:51:45
 Current_time = 21-SEP-2018 19:51:48

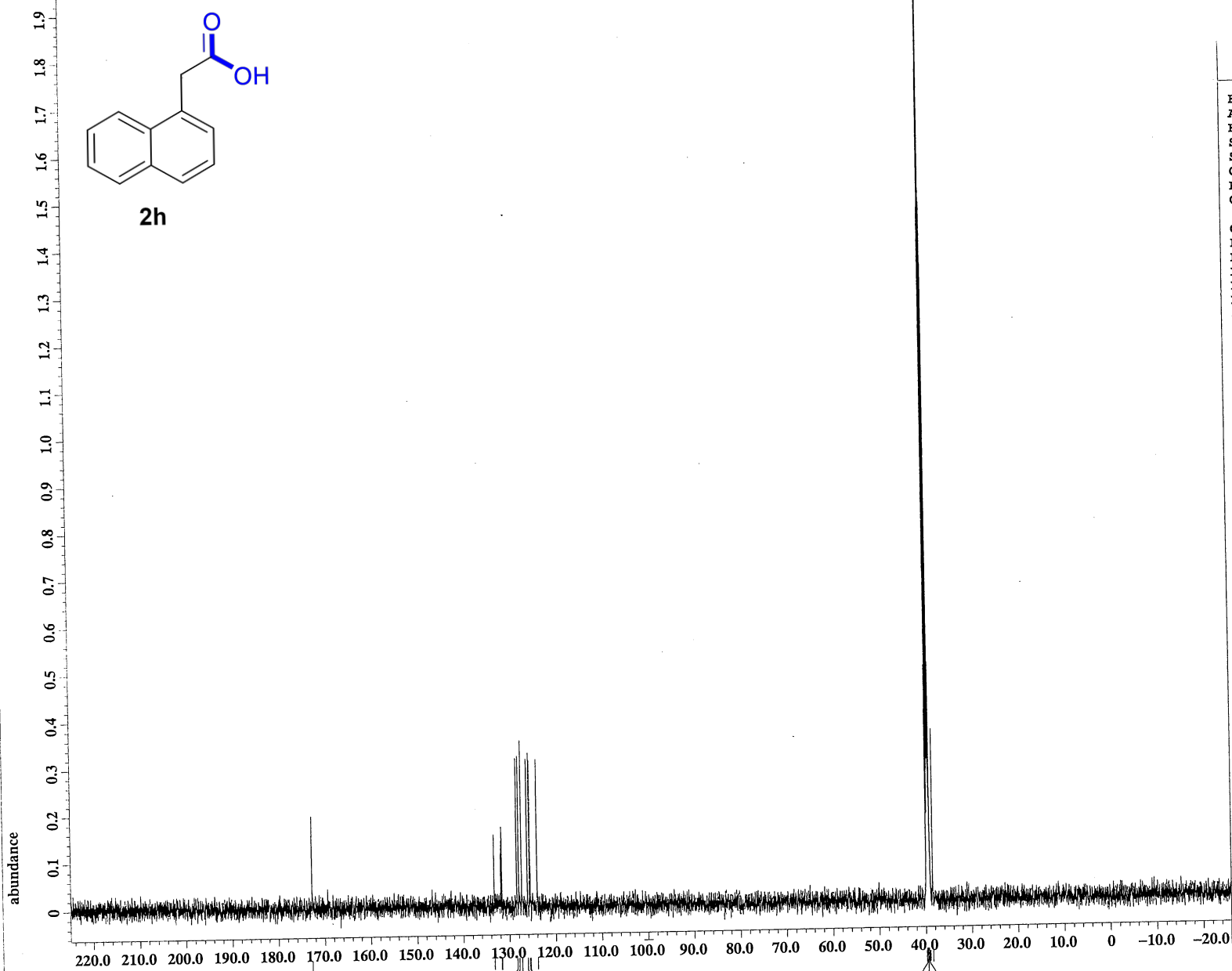
Content = Exp-R-124-1-nap-aceti
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.99090432[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.00917917[Hz]
 X_sweep = 16.53439153[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 12.68[us]
 X_acq_time = 0.99090432[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.34[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.99090432[s]
 Temp_get = 21.3[dC]



2h



172.7816

128.4600
128.0100
127.4068
126.1812
125.7216

39.6636
39.5200
39.3860

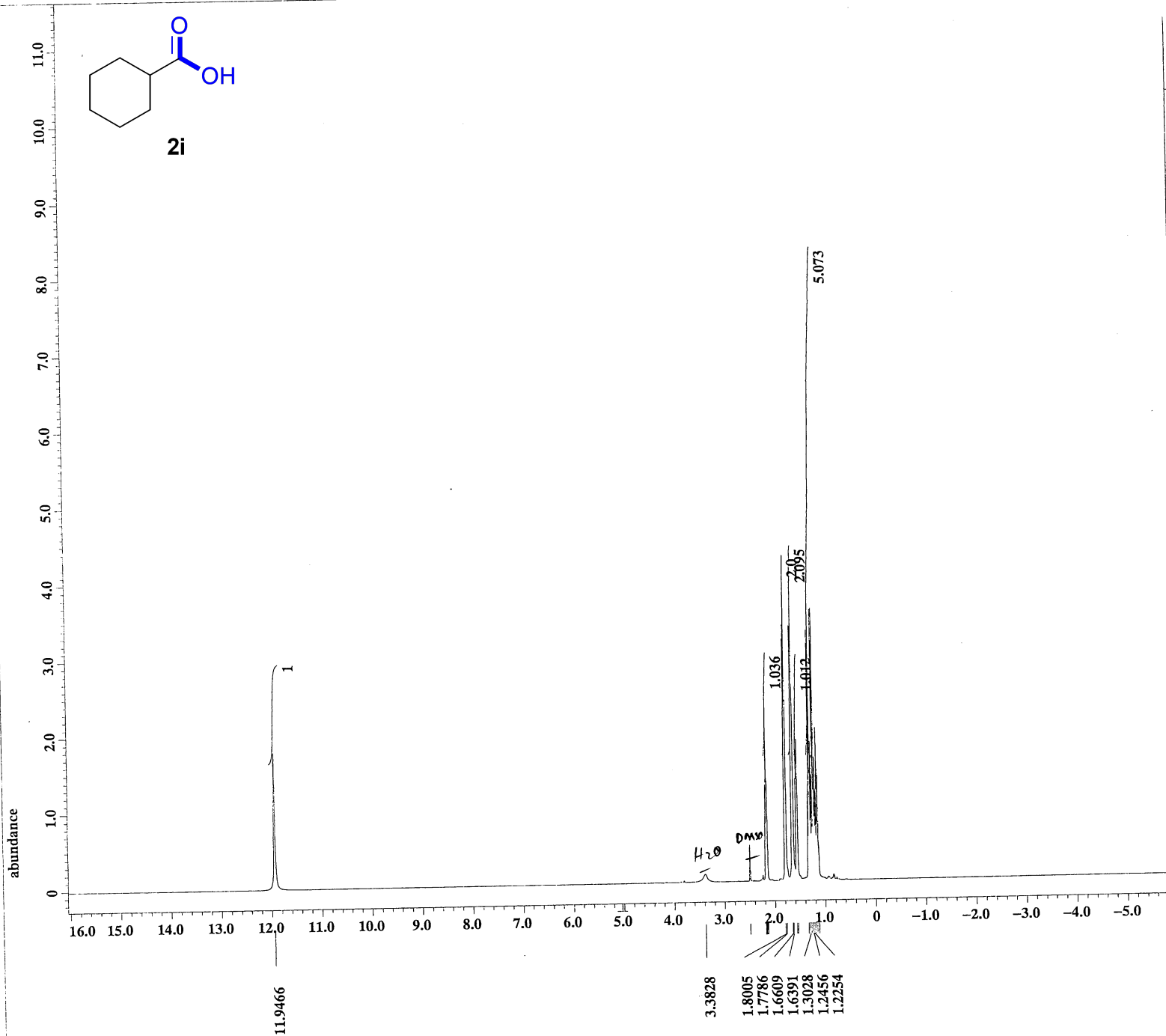
X : parts per Million : 13C

Filename = Exp-R-124-1-nap-aceti
Author = delta
Experiment = single_pulse_dec
Sample_id = Exp-R-124-1-nap-aceti
Solvent = DMSO-D6
Creation_time = 21-SEP-2018 19:46:35
Revision_time = 21-SEP-2018 19:53:37
Current_time = 21-SEP-2018 19:53:58

Content = Exp-R-124-1-nap-aceti
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 60
Total_scans = 60

X_90_width = 12[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 4[us]
Irr_atn_dec = 18.95[dB]
Irr_atn_noe = 18.95[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2.5[s]
Recvr_gain = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get = 22[dc]



```

Filename      = Exp-R-124-5a-proton-4
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-5a-proton
Solvent      = DMSO-D6
Creation_time = 20-SEP-2018 13:05:22
Revision_time = 20-SEP-2018 13:18:43
Current_time  = 20-SEP-2018 13:18:46
  
```

```

Content       = Exp-R-124-5a-proton
Data_format   = 1D_COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 600
Spectrometer  = DELTA2_NMR
  
```

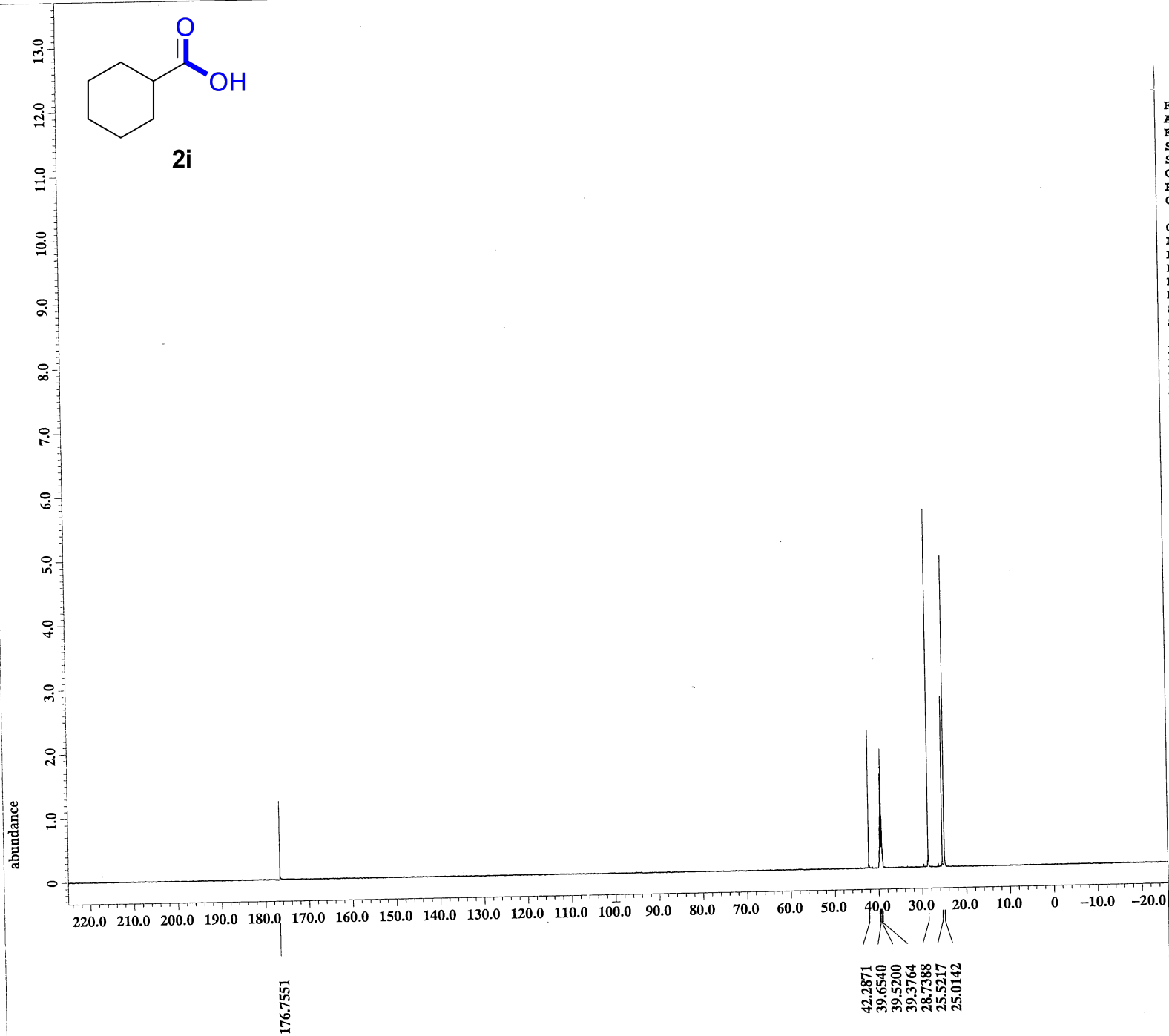
```

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 1.00917917[Hz]
X_sweep        = 16.53439153[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8
  
```

```

X_90_width     = 12.68[us]
X_acq_time      = 0.99090432[s]
X_angle         = 45[deg]
X_atn           = 3.4[db]
X_pulse         = 6.34[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat   = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 32
Relaxation_delay = 5[s]
Repetition_time = 5.99090432[s]
Temp_get        = 22.1[dc]
  
```

X : parts per Million : 1H



```

Filename      = Exp-R-124-5a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-5a-C
Solvent      = DMSO-D6
Creation_time = 20-SEP-2018 13:14:47
Revision_time = 20-SEP-2018 13:21:15
Current_time  = 20-SEP-2018 13:23:00

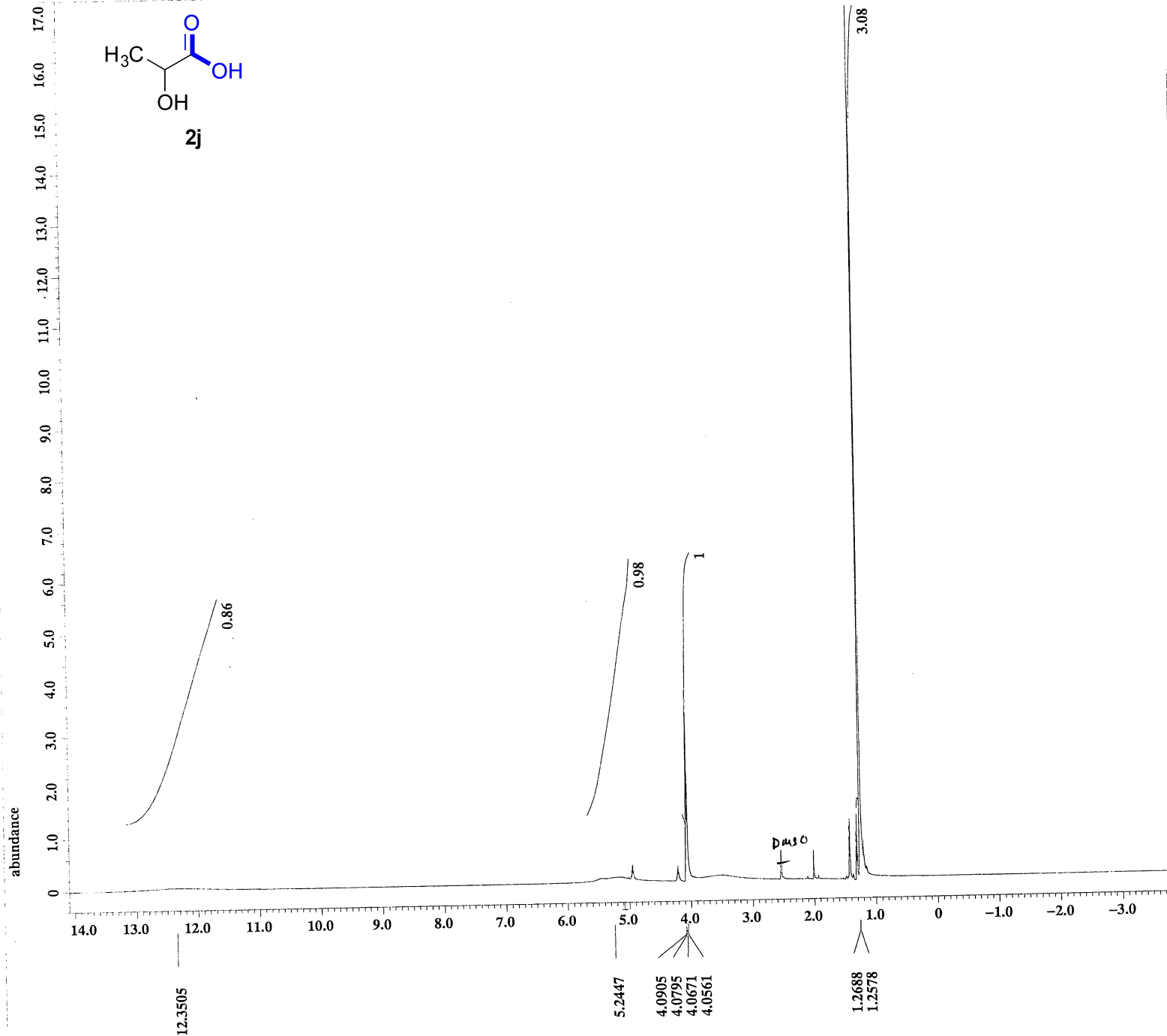
Content      = Exp-R-124-5a-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans    = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 194
Total_scans    = 194

X_90_width    = 12[us]
X_acq_time    = 0.69206016[s]
X_angle       = 30[deg]
X_atn         = 7.5[dB]
X_pulse       = 4[us]
Irr_atn_dec   = 18.95[dB]
Irr_atn_noe   = 18.95[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 2[s]
Recvr_gain    = 60
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get      = 22.3[dC]

```

X : parts per Million : 13C



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

Derived from: Exp-AB-R-124-6c-H-1.jdf

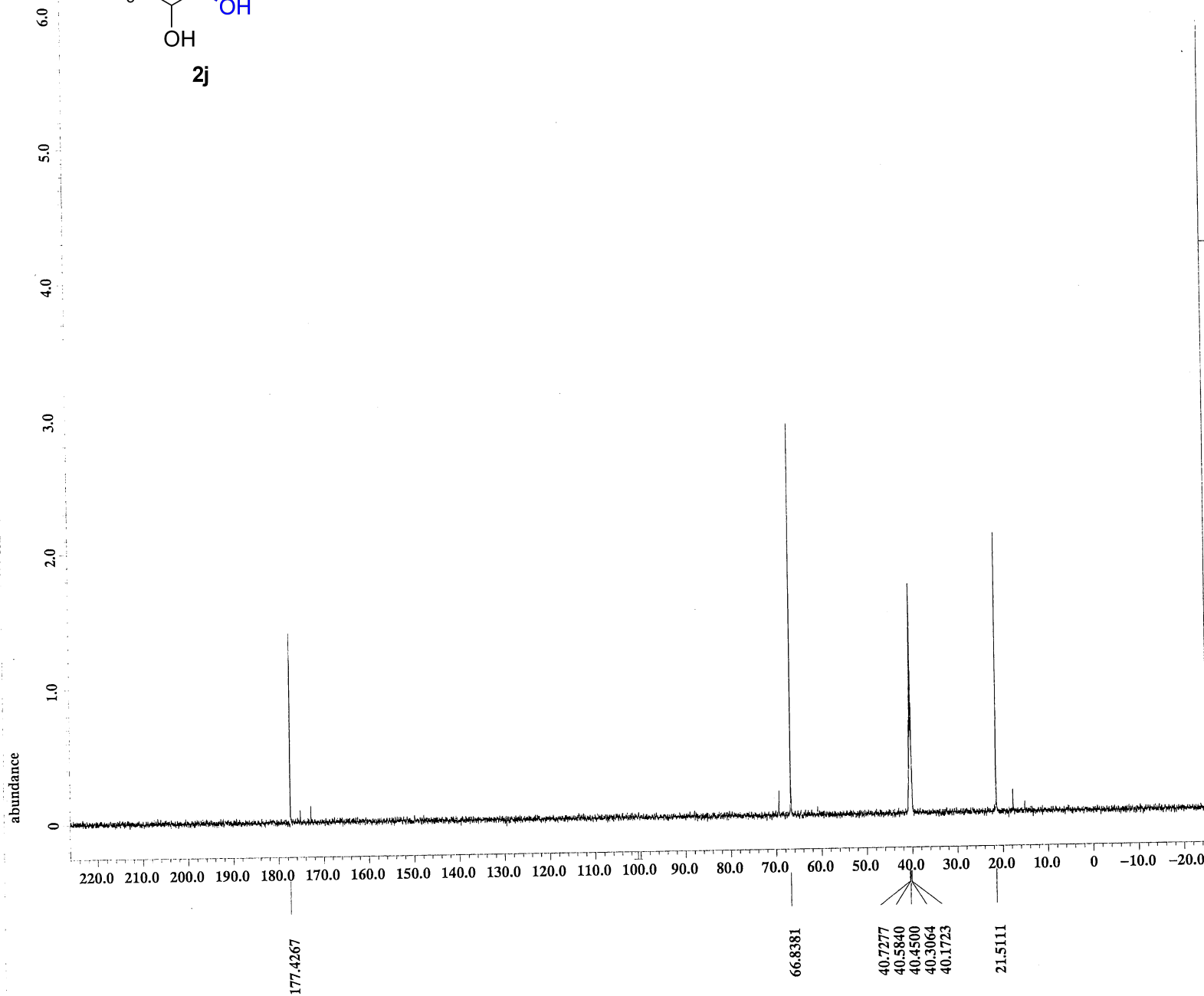
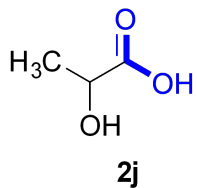
Filename = Exp-AB-R-124-6c-H-5.j
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-AB-R-124-6c-H
 Solvent = DMSO-D6
 Creation_time = 1-SEP-2020 16:21:20
 Revision_time = 2-SEP-2020 13:45:37
 Current_time = 2-SEP-2020 13:45:42

Comment = Exp-AB-R-124-6c-H
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 1.21110528[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.82569205[Hz]
 X_sweep = 13.52813853[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17[us]
 X_acq_time = 1.21110528[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.585[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 36
 Relaxation_delay = 5[s]
 Repetition_time = 6.21110528[s]
 Temp_get = 21.4[dc]

X : parts per Million : 1H



X : parts per Million : 13C

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

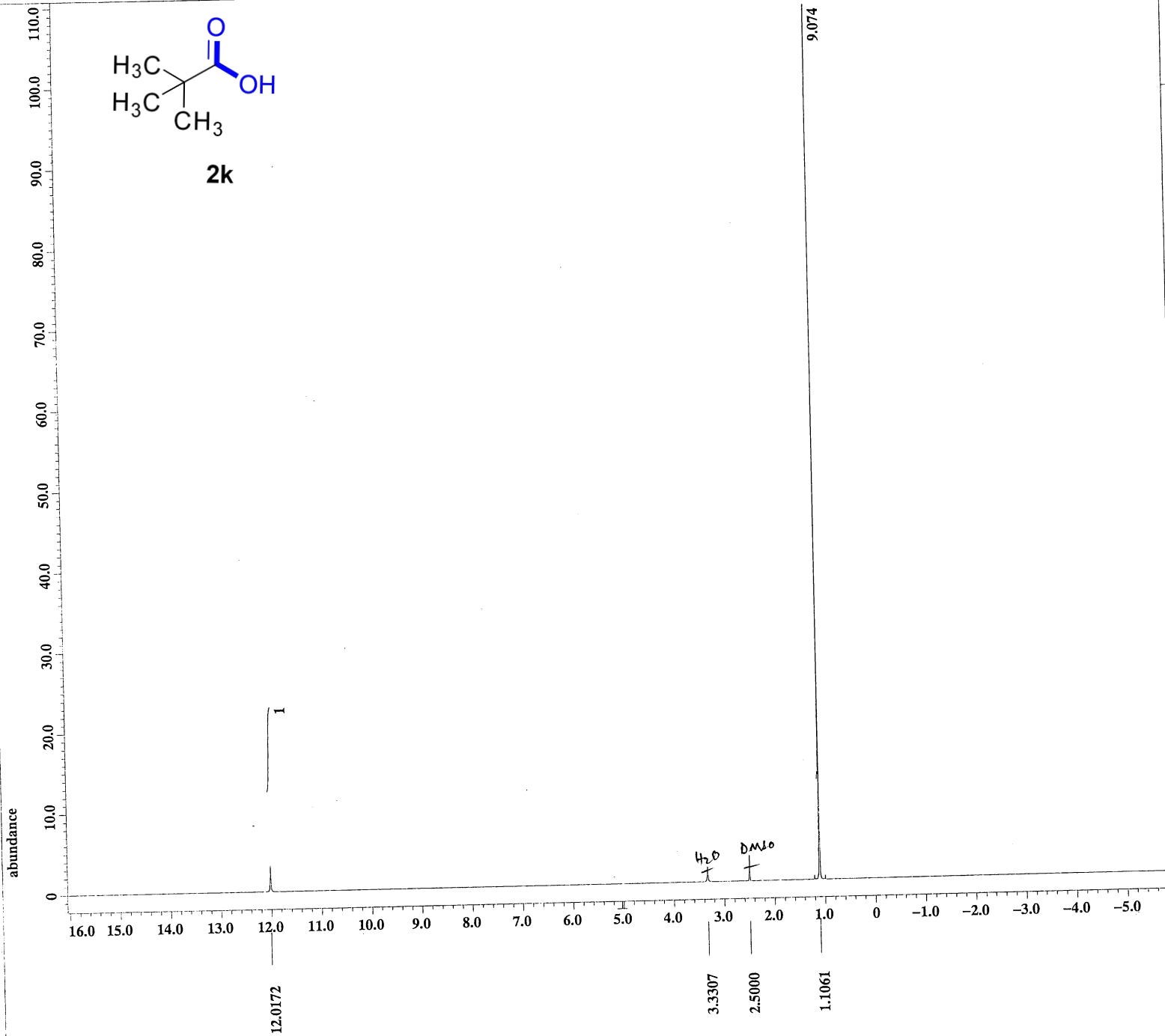
Derived from: Exp-AB-R-124-6c-C-1.jdf

Filename = Exp-AB-R-124-6c-C-4.j
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = Exp-AB-R-124-6c-C
 Solvent = DMSO-D6
 Creation_time = 1-SEP-2020 16:19:40
 Revision_time = 1-SEP-2020 16:26:08
 Current_time = 1-SEP-2020 16:26:22

Comment = Exp-AB-R-124-6c-C
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M])
 X_acq_duration = 0.69206016 [s]
 X_domain = 13C
 X_freq = 150.91343039 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109 [Hz]
 X_sweep = 47.34848485 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 43
 Total_scans = 43

X_90_width = 12.3 [us]
 X_acq_time = 0.69206016 [s]
 X_angle = 30 [deg]
 X_atn = 7.5 [dB]
 X_pulse = 4.1 [us]
 Irr_atn_dec = 18.62 [dB]
 Irr_atn_noe = 18.62 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.69206016 [s]
 Temp_get = 21.7 [dC]



```

Filename      = Exp-R-124-4a-proton-5
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-4a-proton
Solvent      = DMSO-D6
Creation_time = 20-SEP-2018 12:50:42
Revision_time = 20-SEP-2018 13:03:14
Current_time  = 20-SEP-2018 13:03:20
  
```

```

Content       = Exp-R-124-4a-proton
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR
  
```

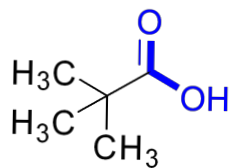
```

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 1.00917917 [Hz]
X_sweep        = 16.53439153 [kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046 [MHz]
Irr_offset     = 5 [ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046 [MHz]
Tri_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8
  
```

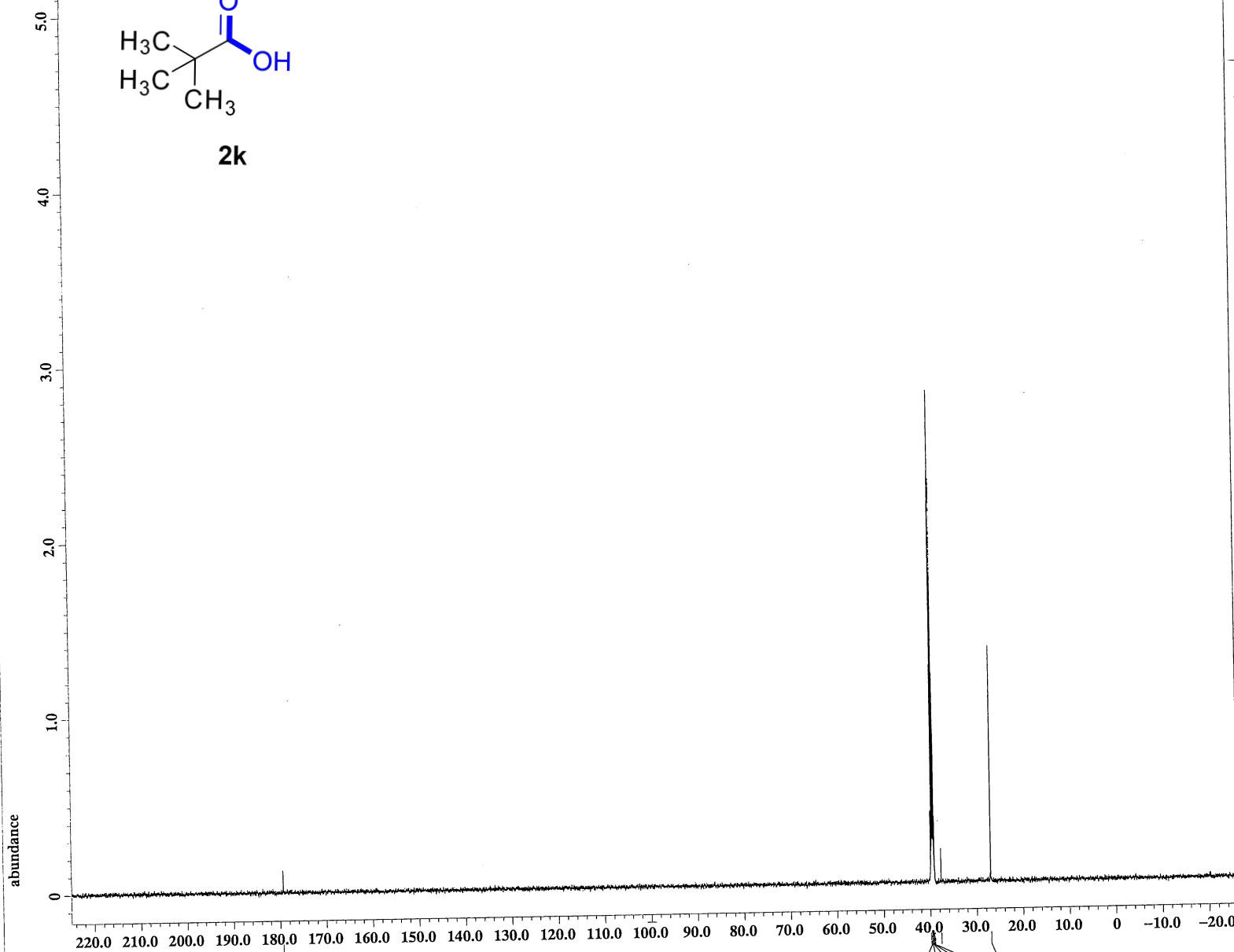
```

X_90_width    = 12.68 [us]
X_acq_time     = 0.99090432 [s]
X_angle        = 45 [deg]
X_atn          = 3.4 [dB]
X_pulse        = 6.34 [us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 48
Relaxation_delay = 5 [s]
Repetition_time = 5.99090432 [s]
Temp_get       = 22.3 [dC]
  
```

X : parts per Million : 1H



2k



X : parts per Million : 13C

```

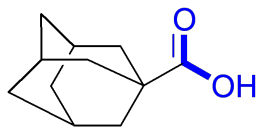
Filename      = Exp-R-124-4a-Carbon-3
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-4a-Carbon
Solvent      = DMSO-D6
Creation_time = 20-SEP-2018 12:57:33
Revision_time = 20-SEP-2018 13:03:57
Current_time  = 20-SEP-2018 13:04:06

Content      = Exp-R-124-4a-Carbon
Data_format  = 1D_COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

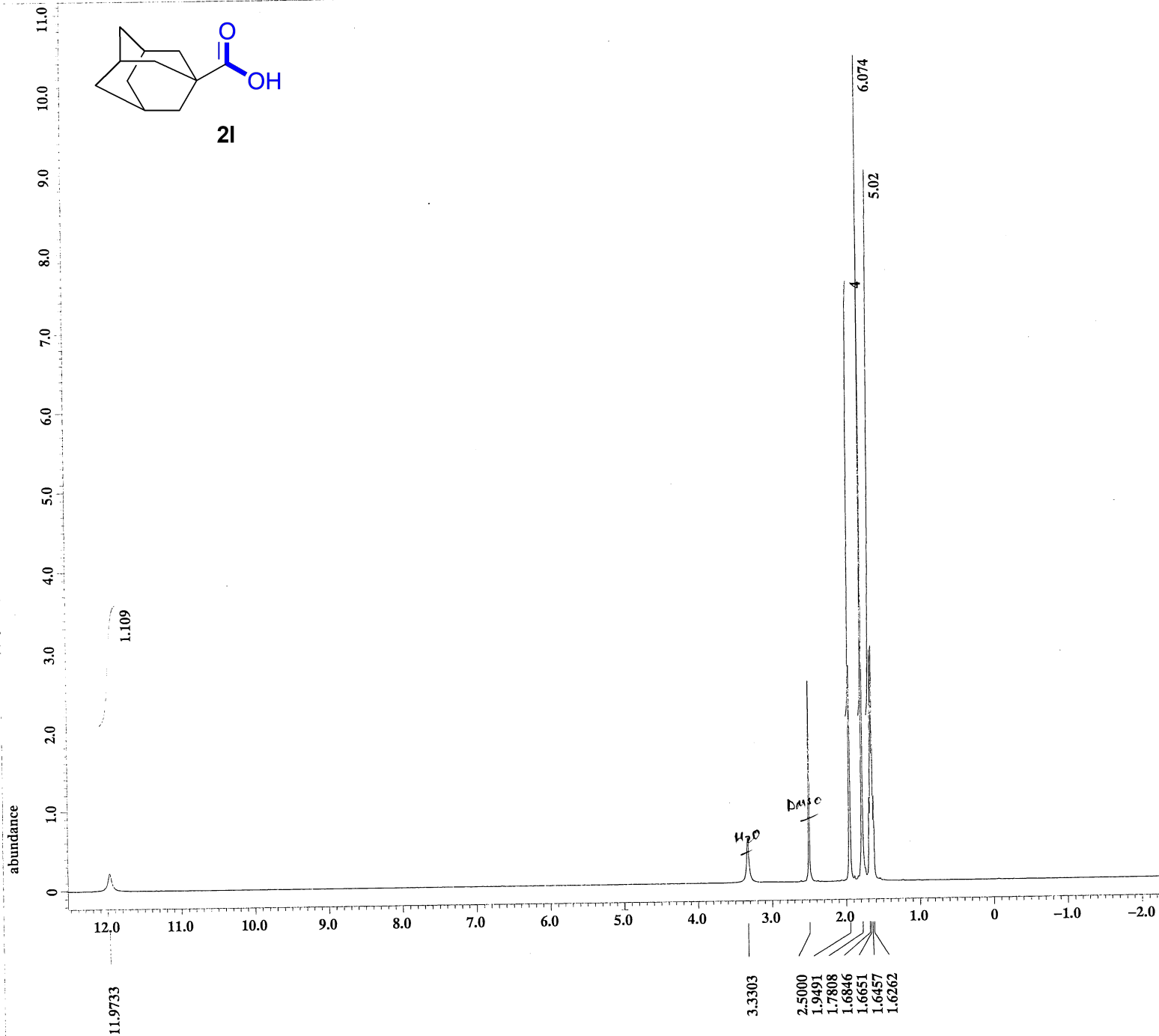
Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 137
Total_scans    = 137

X_90_width    = 12[us]
X_acq_time    = 0.69206016[s]
X_angle       = 30[deg]
X_atn         = 7.5[dB]
X_pulse       = 4[us]
Irr_atn_dec   = 18.95[dB]
Irr_atn_noe   = 18.95[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait   = 1[s]
Noe           = TRUE
Noe_time      = 2[s]
Recvr_gain    = 60
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get      = 22.4[dC]

```



21



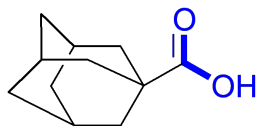
X : parts per Million : 1H

Filename = Exp-R-122-3aDMSO-P-4.
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-122-3aDMSO-P
 Solvent = DMSO-D6
 Creation_time = 31-JUL-2018 18:14:27
 Revision_time = 31-JUL-2018 18:47:30
 Current_time = 31-JUL-2018 18:47:39

Content = Exp-R-122-3aDMSO-P
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

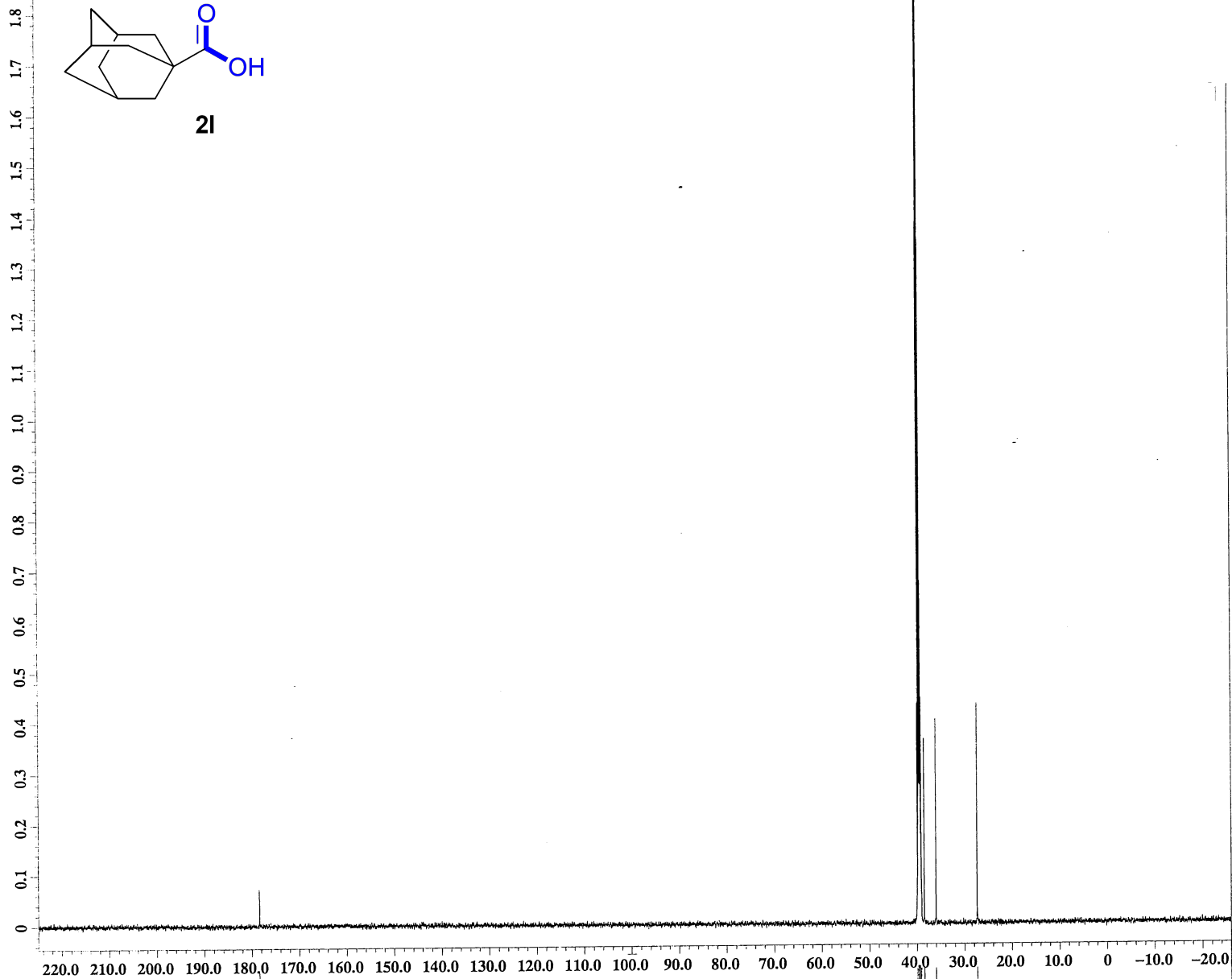
Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 1.4548992[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.68733284[Hz]
 X_sweep = 11.26126126[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 12.68[us]
 X_acq_time = 1.4548992[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.34[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 6.4548992[s]
 Temp_get = 21.8[dC]



21

abundance



178.4402

39.9317
39.7977
39.6540
39.5200
39.3764
39.2423

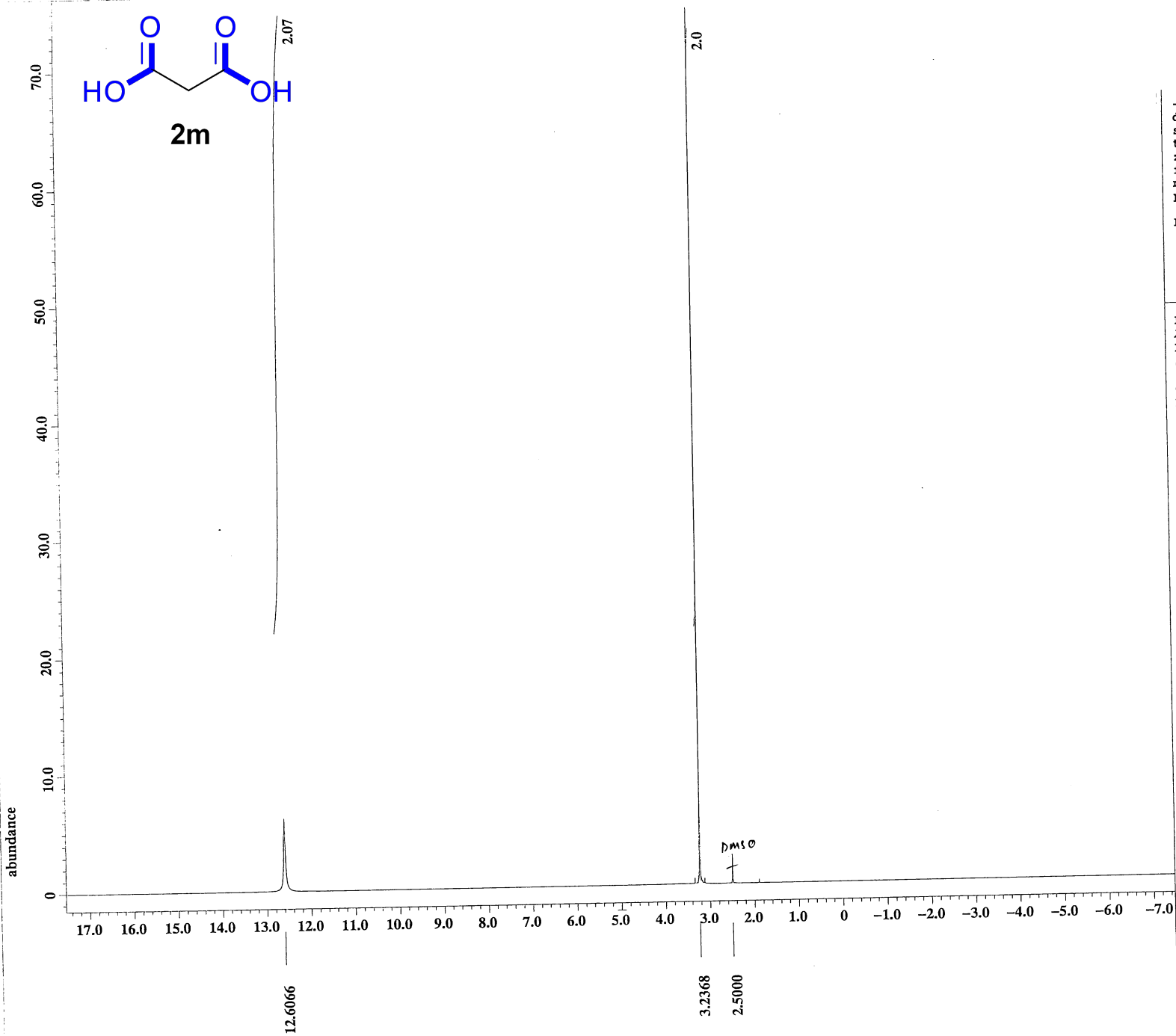
X : parts per Million : 13C

Filename = Exp-R-122-3aDMSO-Carb
Author = delta
Experiment = single_pulse_dec
Sample_id = Exp-R-122-3aDMSO-Carb
Solvent = DMSO-D6
Creation_time = 31-JUL-2018 19:11:45
Revision_time = 31-JUL-2018 19:42:14
Current_time = 31-JUL-2018 19:42:29

Content = Exp-R-122-3aDMSO-Carb
Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M])
X_acq_duration = 0.69206016 [s]
X_domain = 13C
X_freq = 150.91343039 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109 [Hz]
X_sweep = 47.34848485 [kHz]
Irr_domain = 1H
Irr_freq = 600.1723046 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 914
Total_scans = 914

X_90_width = 12 [us]
X_acq_time = 0.69206016 [s]
X_angle = 30 [deg]
X_atn = 7.5 [dB]
X_pulse = 4 [us]
Irr_atn_dec = 18.95 [dB]
Irr_atn_noe = 18.95 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2.5 [s]
Recvr_gain = 60
Relaxation_delay = 2.5 [s]
Repetition_time = 3.19206016 [s]
Temp_get = 22.5 [dC]



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

Derived from: Exp-R-184-5-P-1.jdf

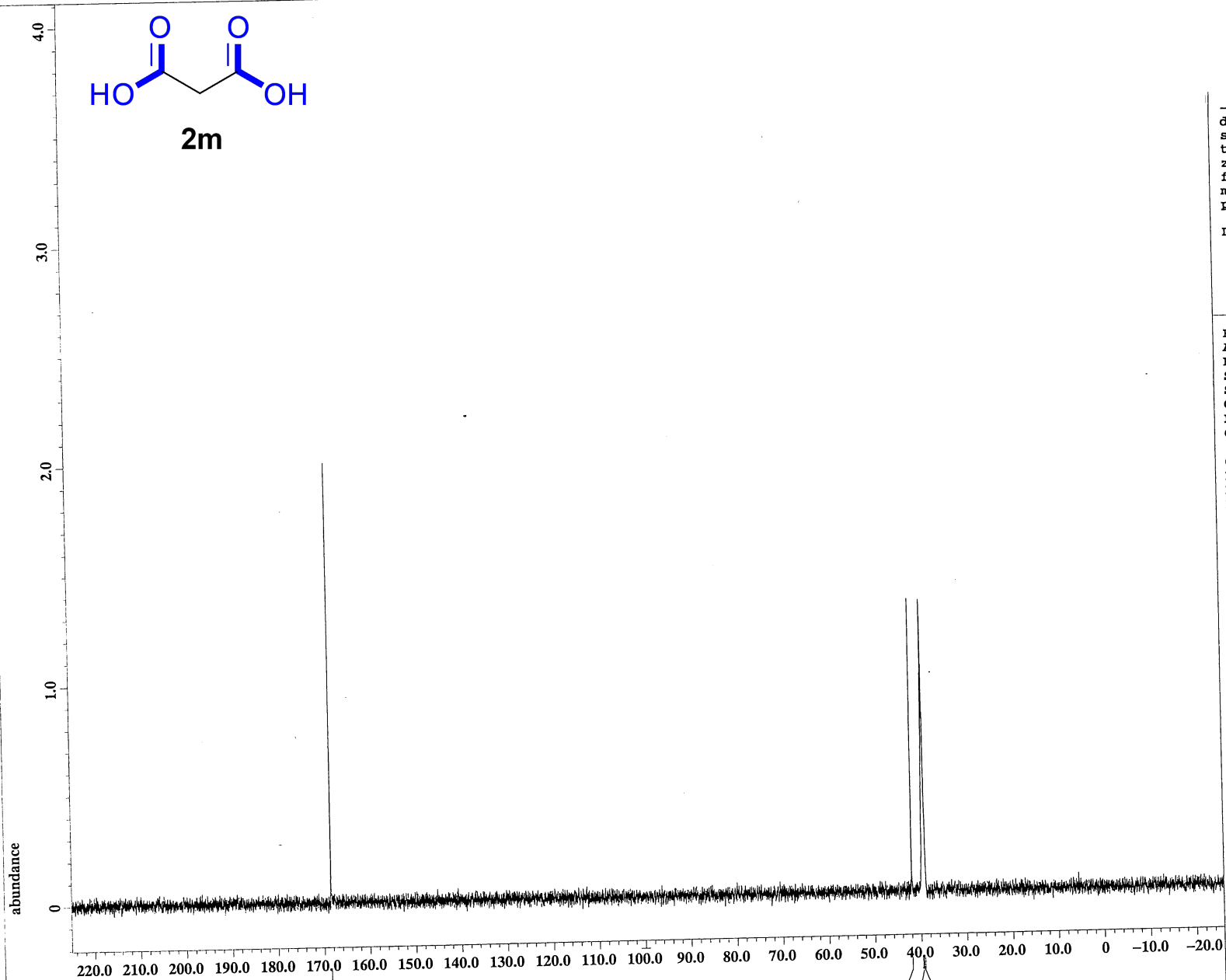
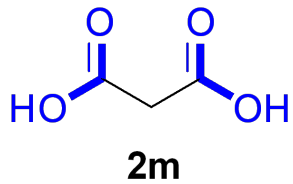
Filename = Exp-R-184-5-P-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-184-5-P
 Solvent = DMSO-D6
 Creation_time = 18-APR-2019 16:43:32
 Revision_time = 18-APR-2019 16:49:30
 Current_time = 18-APR-2019 16:49:36

Comment = Exp-R-184-5-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.87293952[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.14555473[Hz]
 X_sweep = 18.76876877[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17[us]
 X_acq_time = 0.87293952[s]
 X_angle = 45[deg]
 X_atn = 3.4[db]
 X_pulse = 6.585[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 44
 Relaxation_delay = 5[s]
 Repetition_time = 5.87293952[s]
 Temp_get = 21.5[dc]

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: Exp-R-184-5-C-1.jdf

```

```

Filename      = Exp-R-184-5-C-3.jdf
Author       = delta
Experiment    = single_pulse_dec
Sample_id     = Exp-R-184-5-C
Solvent      = DMSO-D6
Creation_time = 18-APR-2019 16:45:24
Revision_time = 18-APR-2019 16:50:30
Current_time  = 18-APR-2019 16:50:44

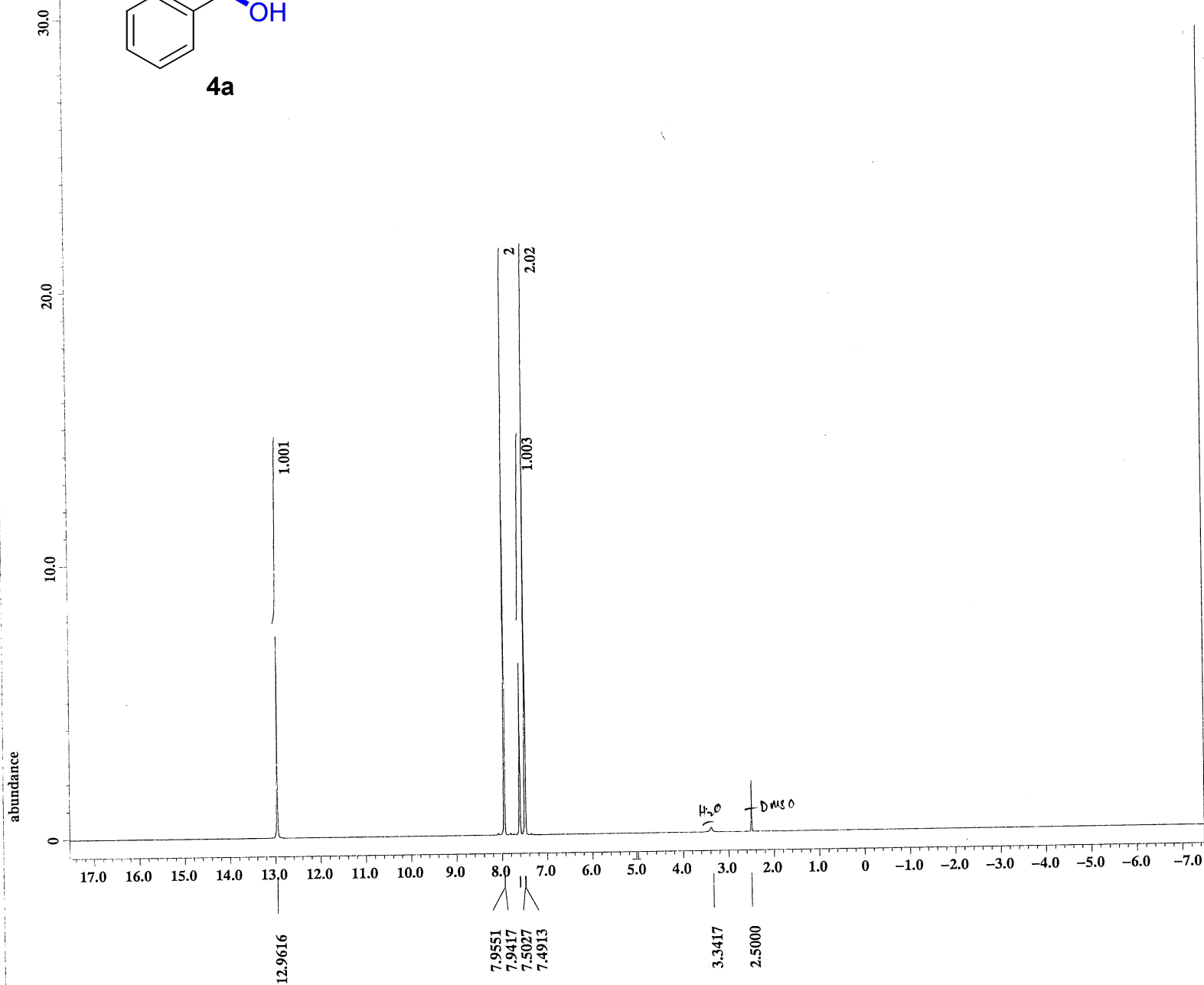
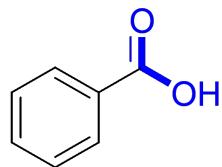
Comment      = Exp-R-184-5-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109 [Hz]
X_sweep        = 47.34848485 [kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046 [MHz]
Irr_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 26
Total_scans    = 26

X_90_width     = 12.7 [us]
X_acq_time     = 0.69206016 [s]
X_angle        = 30 [deg]
X_atn          = 7.5 [dB]
X_pulse        = 4.23333333 [us]
Irr_atn_dec    = 18.62 [dB]
Irr_atn_noe    = 18.62 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.69206016 [s]
Temp_get       = 21.5 [dC]

```

X : parts per Million : 13C



X : parts per Million : 1H

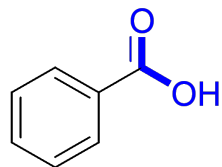
```

Filename      = Exp-R-124-28b-P-5.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-28b-P
Solvent      = DMSO-D6
Creation_time = 29-AUG-2018 20:27:04
Revision_time = 29-AUG-2018 21:20:46
Current_time  = 29-AUG-2018 21:20:50

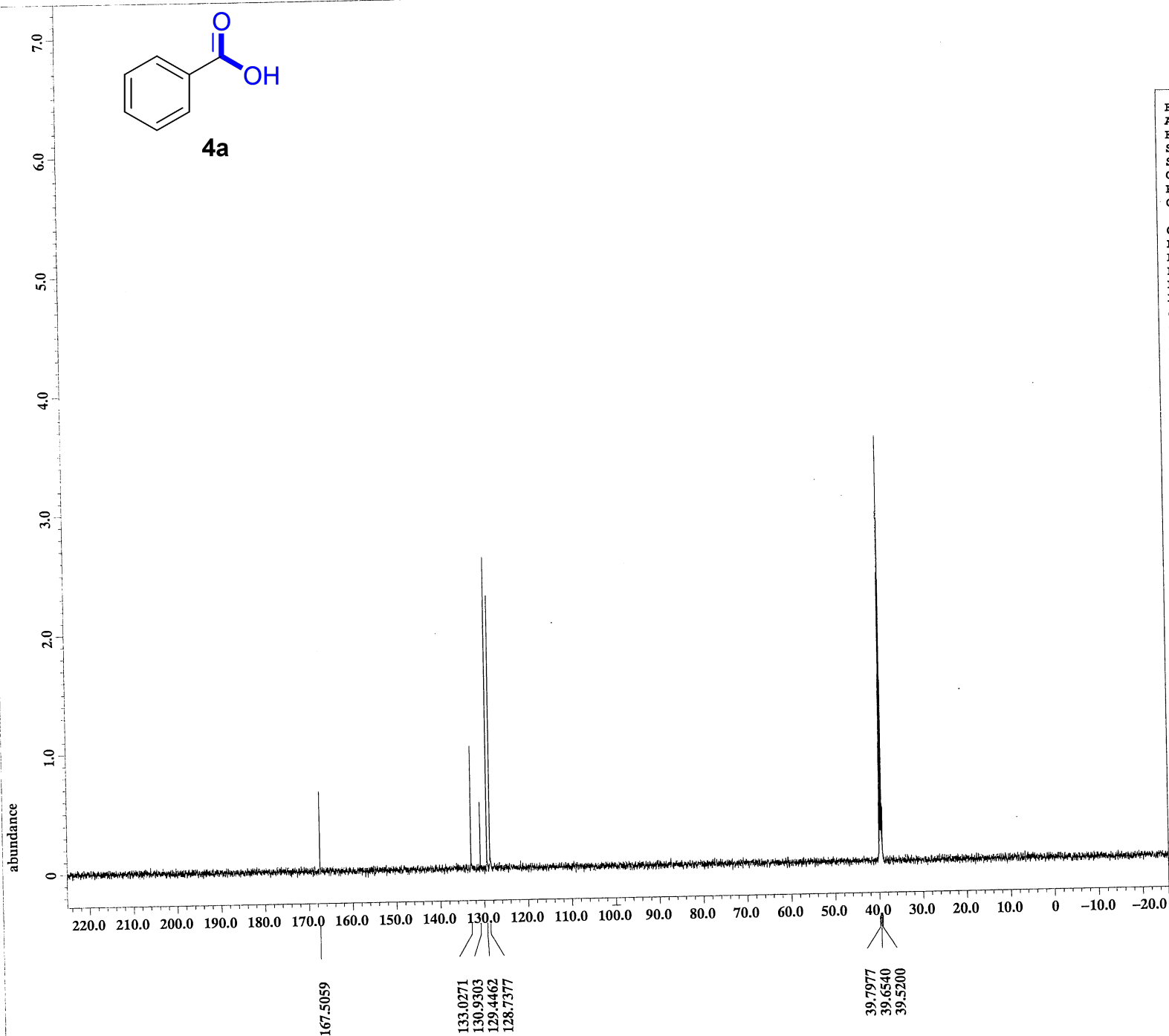
Content      = Exp-R-124-28b-P
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600[M]
X_acq_duration = 0.87293952 [s]
X_domain       = 1H
X_freq         = 600.1723046 [MHz]
X_offset       = 5 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 1.14555473 [Hz]
X_sweep        = 18.76876877 [kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046 [MHz]
Irr_offset     = 5 [ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046 [MHz]
Tri_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 12.68 [us]
X_acq_time     = 0.87293952 [s]
X_angle        = 45 [deg]
X_atn          = 3.4 [dB]
X_pulse        = 6.34 [us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 44
Relaxation_delay = 5 [s]
Repetition_time = 5.87293952 [s]
Temp_get       = 21.4 [dC]
  
```

4a



X : parts per Million : 13C

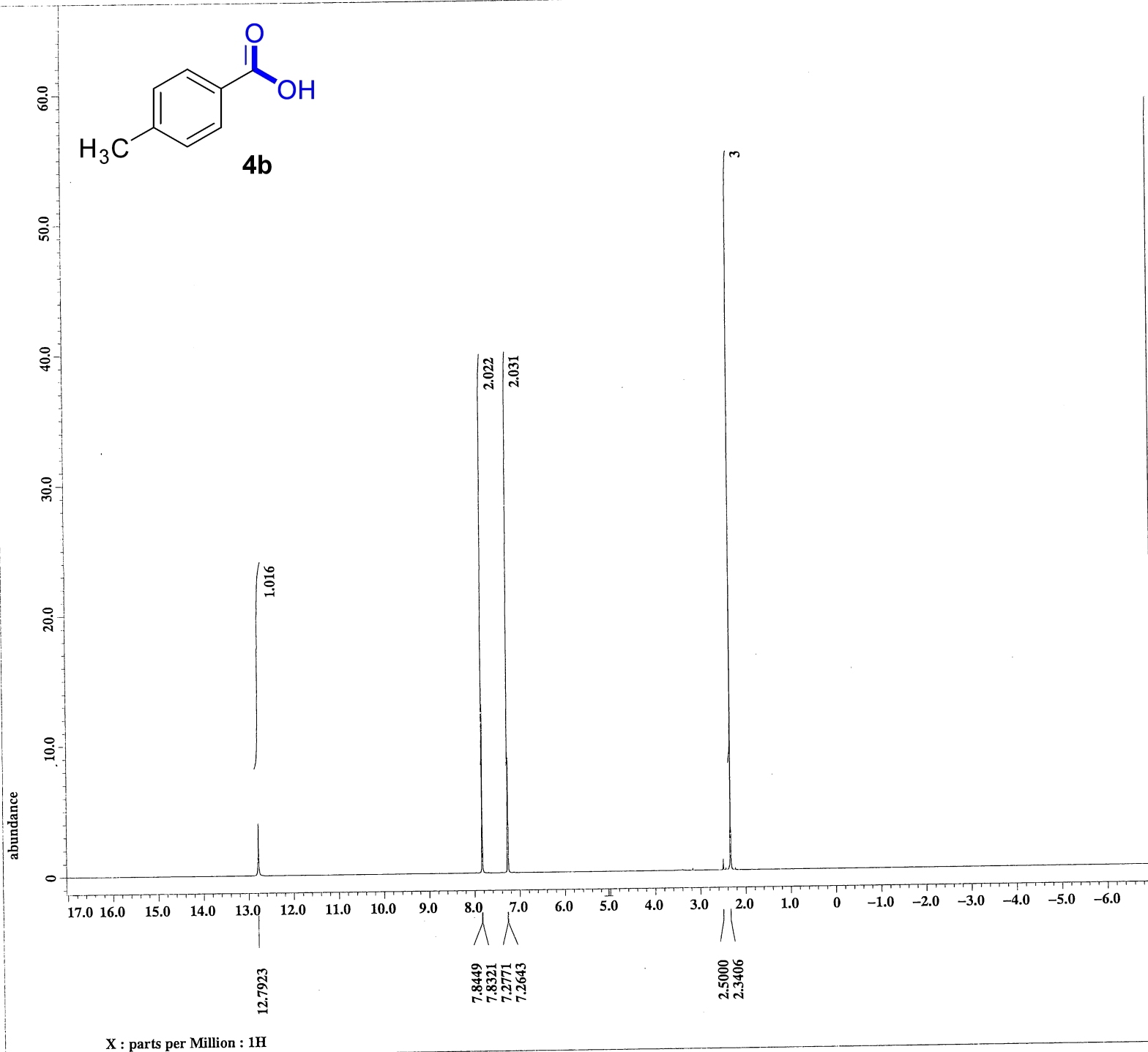
```

Filename      = Exp-R-124-28b-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-28b-C
Solvent      = DMSO-D6
Creation_time = 29-AUG-2018 21:19:34
Revision_time = 29-AUG-2018 21:21:41
Current_time  = 29-AUG-2018 21:22:01

Content      = Exp-R-124-28b-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq        = 150.91343039[MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution   = 1.44496109 [Hz]
X_sweep       = 47.34848485 [kHz]
Irr_domain    = 1H
Irr_freq      = 600.1723046 [MHz]
Irr_offset    = 5 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 27
Total_scans   = 27

X_90_width    = 12 [us]
X_acq_time    = 0.69206016 [s]
X_angle       = 30 [deg]
X_atn         = 7.5 [dB]
X_pulse       = 4 [us]
Irr_atn_dec   = 18.95 [dB]
Irr_atn_noe   = 18.95 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 2.5 [s]
Recvr_gain    = 60
Relaxation_delay = 2.5 [s]
Repetition_time = 3.19206016 [s]
Temp_get      = 22.2 [dC]
  
```

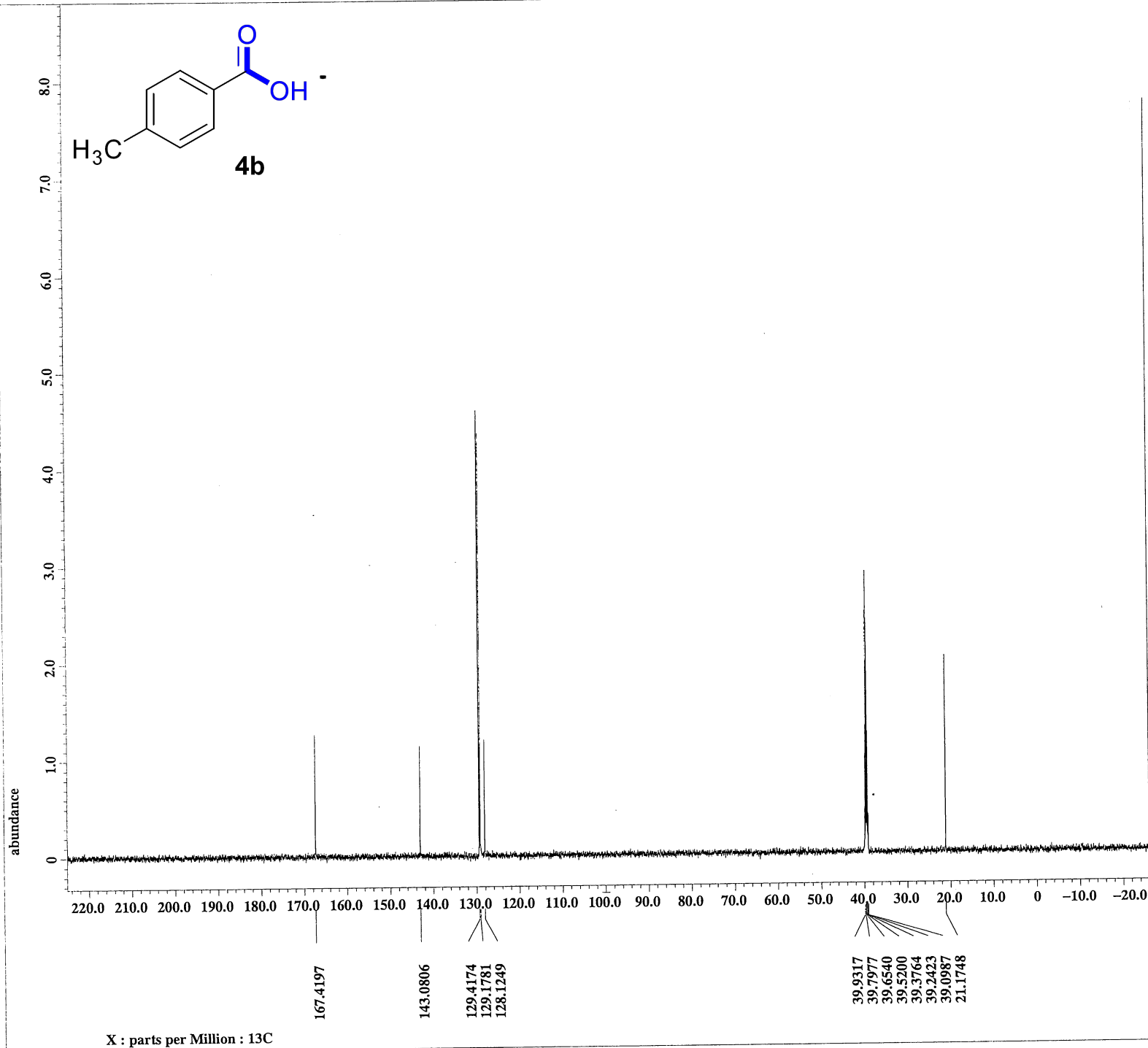


Filename = Exp-R-124-14a-P-6.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-124-14a-P
 Solvent = DMSO-D6
 Creation_time = 25-SEP-2018 19:22:16
 Revision_time = 25-SEP-2018 19:31:43
 Current_time = 25-SEP-2018 19:31:45

Content = Exp-R-124-14a-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.90963968[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.09933639[Hz]
 X_sweep = 18.01152738[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 12.68[us]
 X_acq_time = 0.90963968[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.34[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 36
 Relaxation_delay = 5[s]
 Repetition_time = 5.90963968[s]
 Temp_get = 21.7[dc]



```

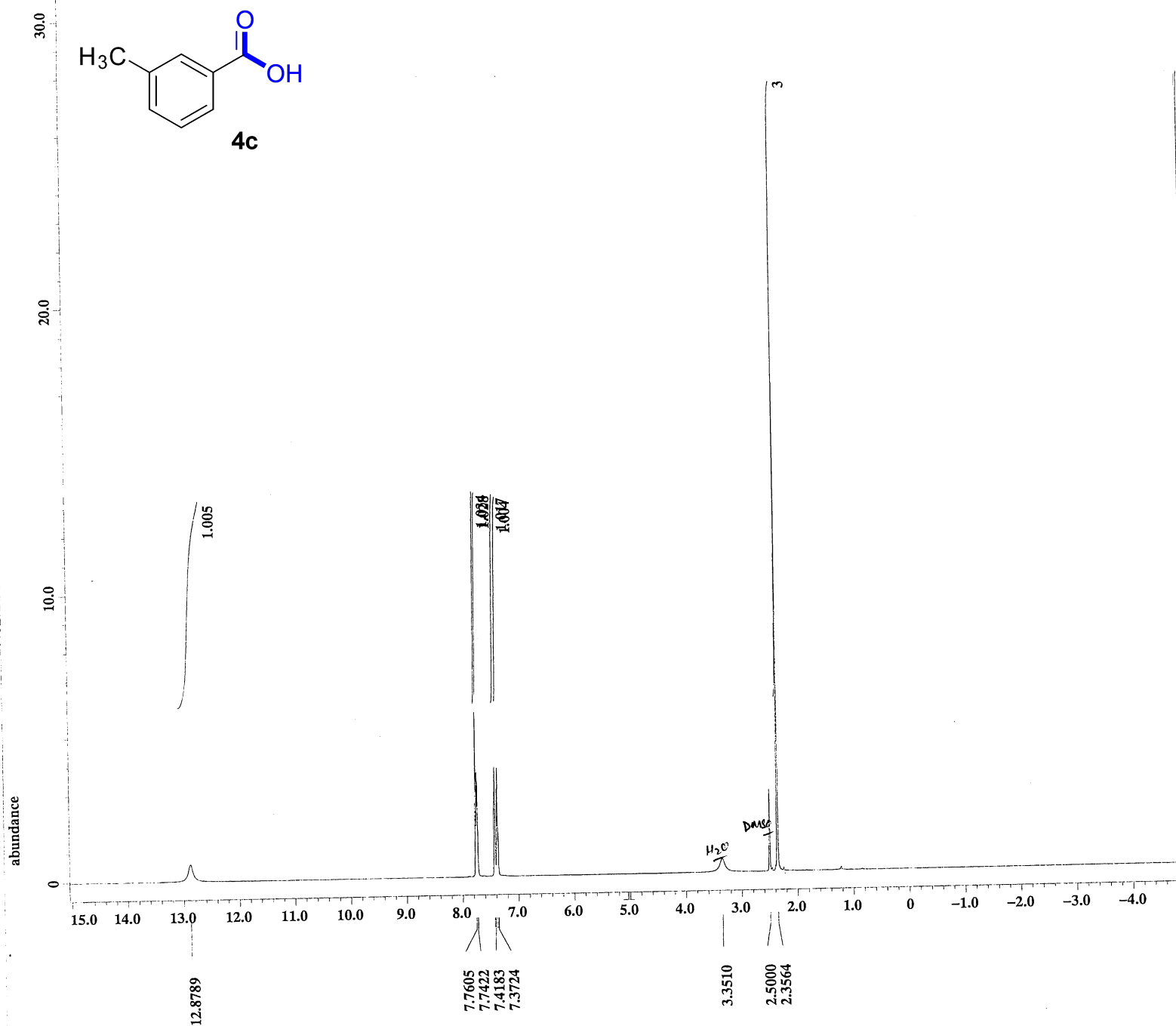
Filename      = Exp-R-124-14a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-14a-C
Solvent      = DMSO-D6
Creation_time = 25-SEP-2018 19:20:35
Revision_time = 25-SEP-2018 19:27:15
Current_time  = 25-SEP-2018 19:27:57

Content      = Exp-R-124-14a-C
Data_format  = 1D_COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = TRUE
Mod_return     = 1
Scans          = 23
Total_scans    = 23

X_90_width    = 12[us]
X_acq_time    = 0.69206016[s]
X_angle       = 30[deg]
X_atn         = 7.5[dB]
X_pulse       = 4[us]
Irr_atn_dec   = 18.95[dB]
Irr_atn_noe   = 18.95[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 2.5[s]
Recvr_gain    = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get      = 21.8[dC]

```



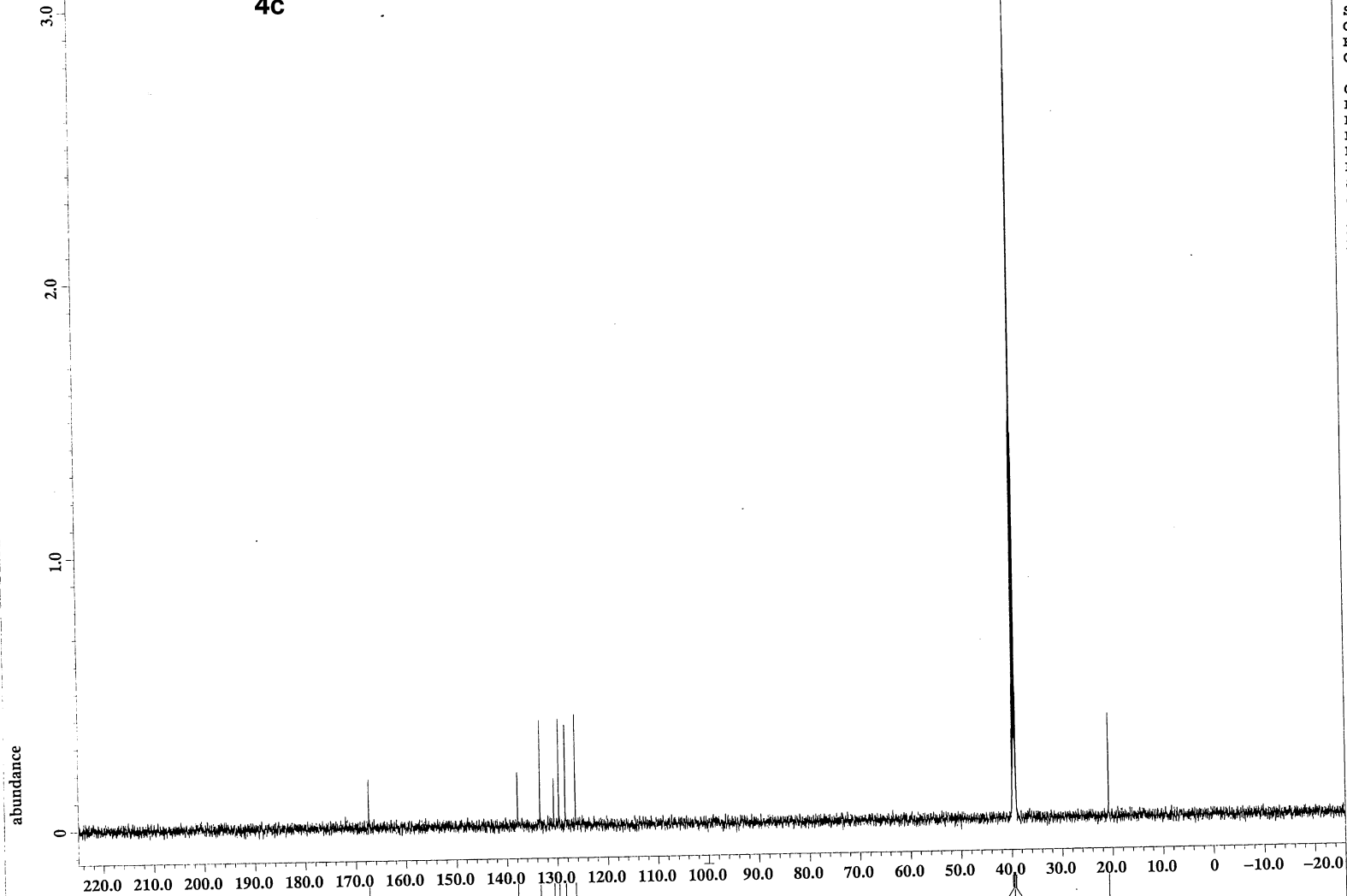
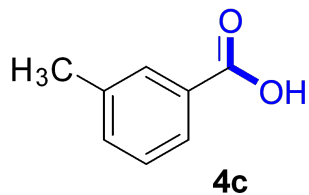
Filename = Exp-R-122-1a-P-6.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-122-1a-P
 Solvent = DMSO-D6
 Creation_time = 1-AUG-2018 18:28:10
 Revision_time = 1-AUG-2018 18:59:58
 Current_time = 1-AUG-2018 19:00:03

Content = Exp-R-122-1a-P
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 1.09051904[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.91699454[Hz]
 X_sweep = 15.02403846[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 12.68[us]
 X_acq_time = 1.09051904[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.34[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 6.09051904[s]
 Temp_get = 22[dc]

X : parts per Million : 1H



167.4293

137.9007
133.4676
130.7483
129.7430
128.4695
126.4684

39.6540
39.5200
39.3764

20.8205

X : parts per Million : 13C

```

Filename      = Exp-R-122-1a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-122-1a-C
Solvent      = DMSO-D6
Creation_time = 1-AUG-2018 18:26:24
Revision_time = 1-AUG-2018 19:02:34
Current_time  = 1-AUG-2018 19:03:06
  
```

```

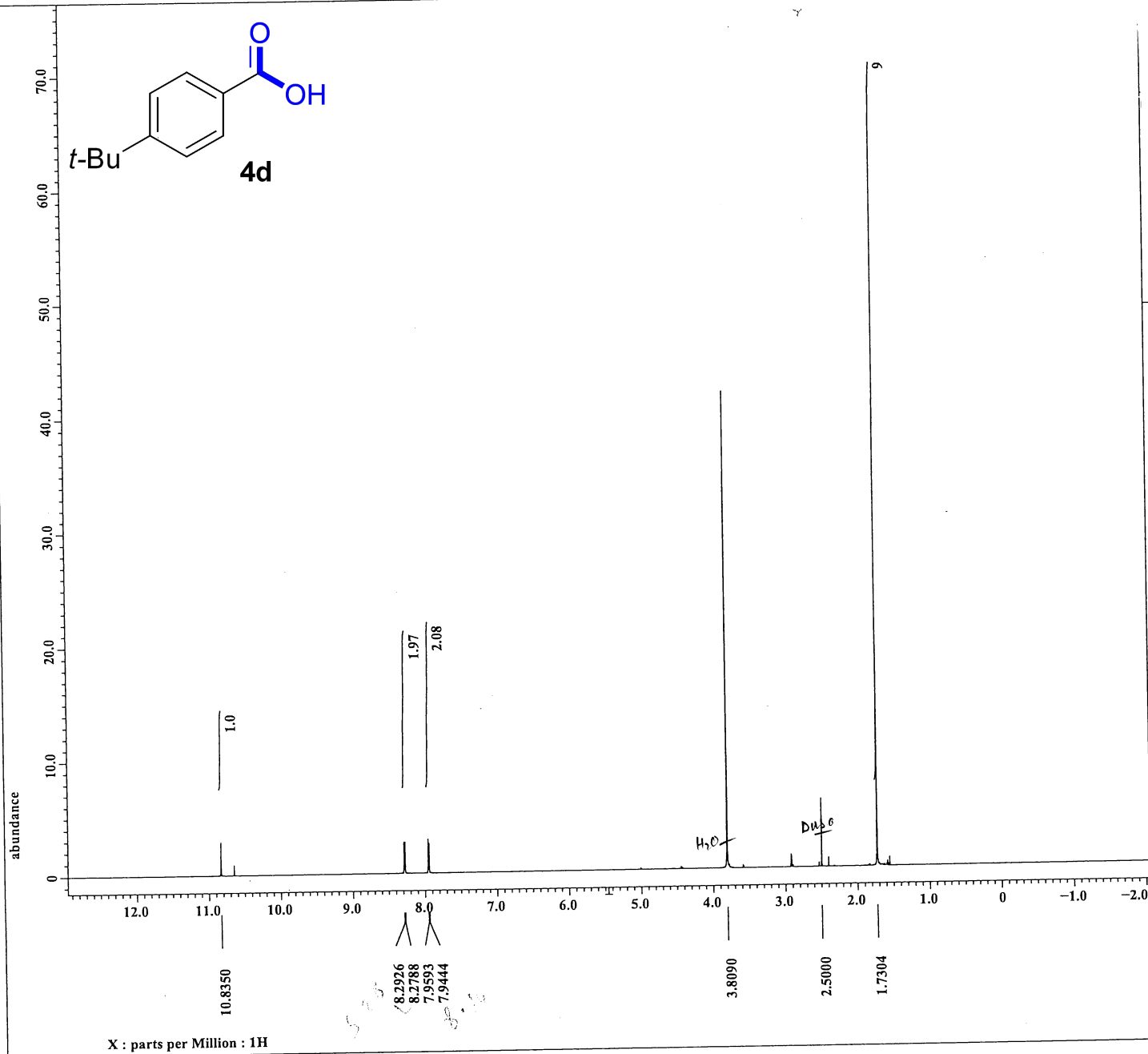
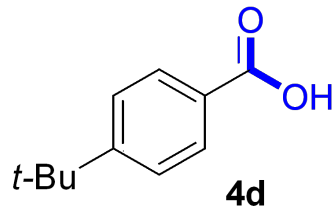
Content      = Exp-R-122-1a-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR
  
```

```

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 52
Total_scans    = 52
  
```

```

X_90_width    = 12[us]
X_acq_time     = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 7.5[dB]
X_pulse        = 4[us]
Irr_atn_dec    = 18.95[dB]
Irr_atn_noe    = 18.95[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2.5[s]
Recvr_gain     = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get       = 22.3[degC]
  
```



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

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

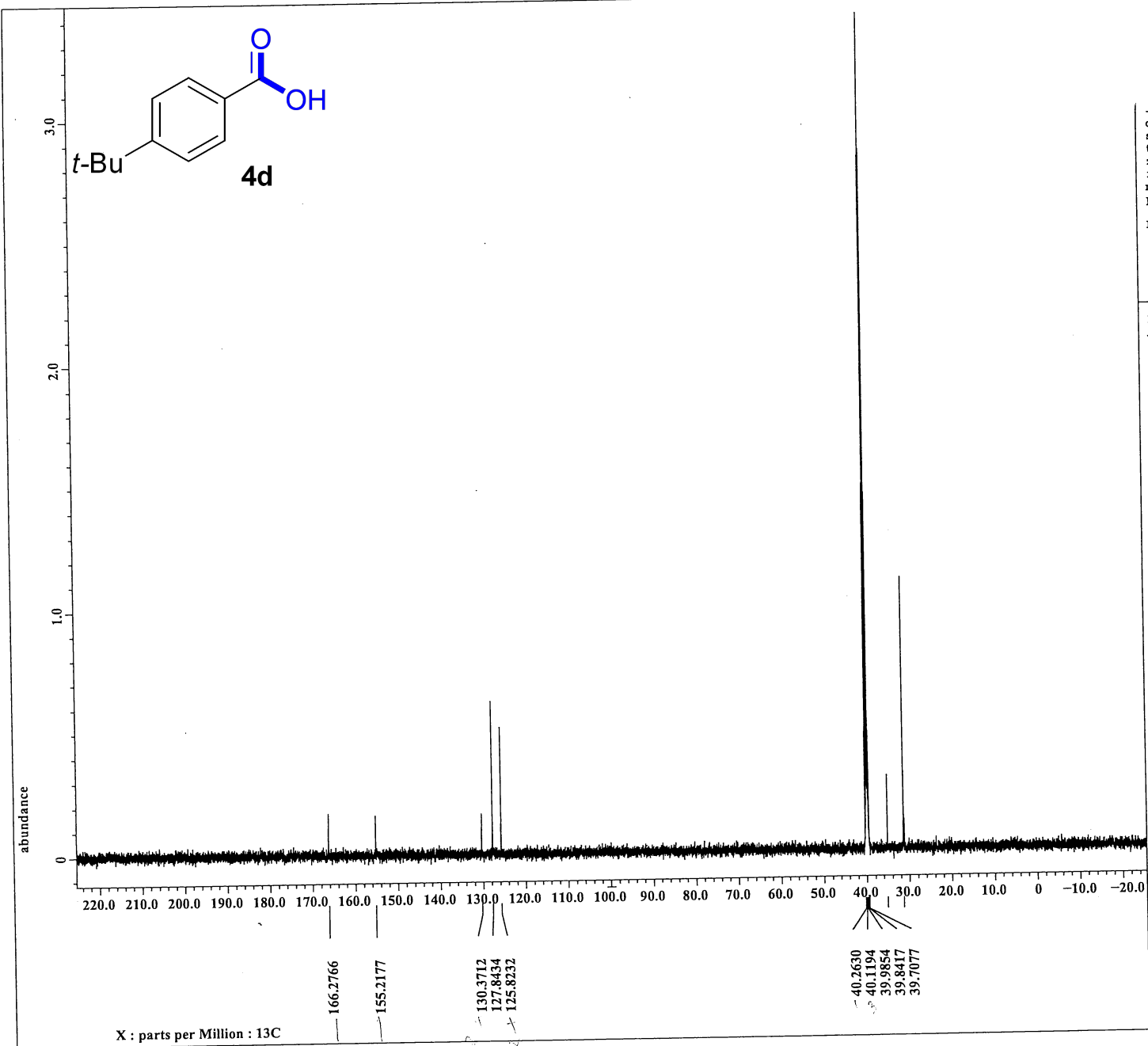
Derived from: Exp-R-165-17-1b-P-1.jdf

Filename = Exp-R-165-17-1b-P-4.j
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-165-17-1b-P
 Solvent = DMSO-D6
 Creation_time = 25-DEC-2018 20:12:18
 Revision_time = 25-DEC-2018 20:16:48
 Current_time = 25-DEC-2018 20:20:08

Comment = Exp-R-165-17-1b-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M
 X_acq_duration = 1.4548992 [s]
 X_domain = 1H
 X_freq = 600.1723046 [MHz]
 X_offset = 5 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.68733284 [Hz]
 X_sweep = 11.26126126 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17 [us]
 X_acq_time = 1.4548992 [s]
 X_angle = 45 [deg]
 X_atn = 3.4 [dB]
 X_atn = 6.585 [us]
 X_pulse = Off
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 40
 Relaxation_delay = 5 [s]
 Repetition_time = 6.4548992 [s]
 Temp_get = 20 [dC]



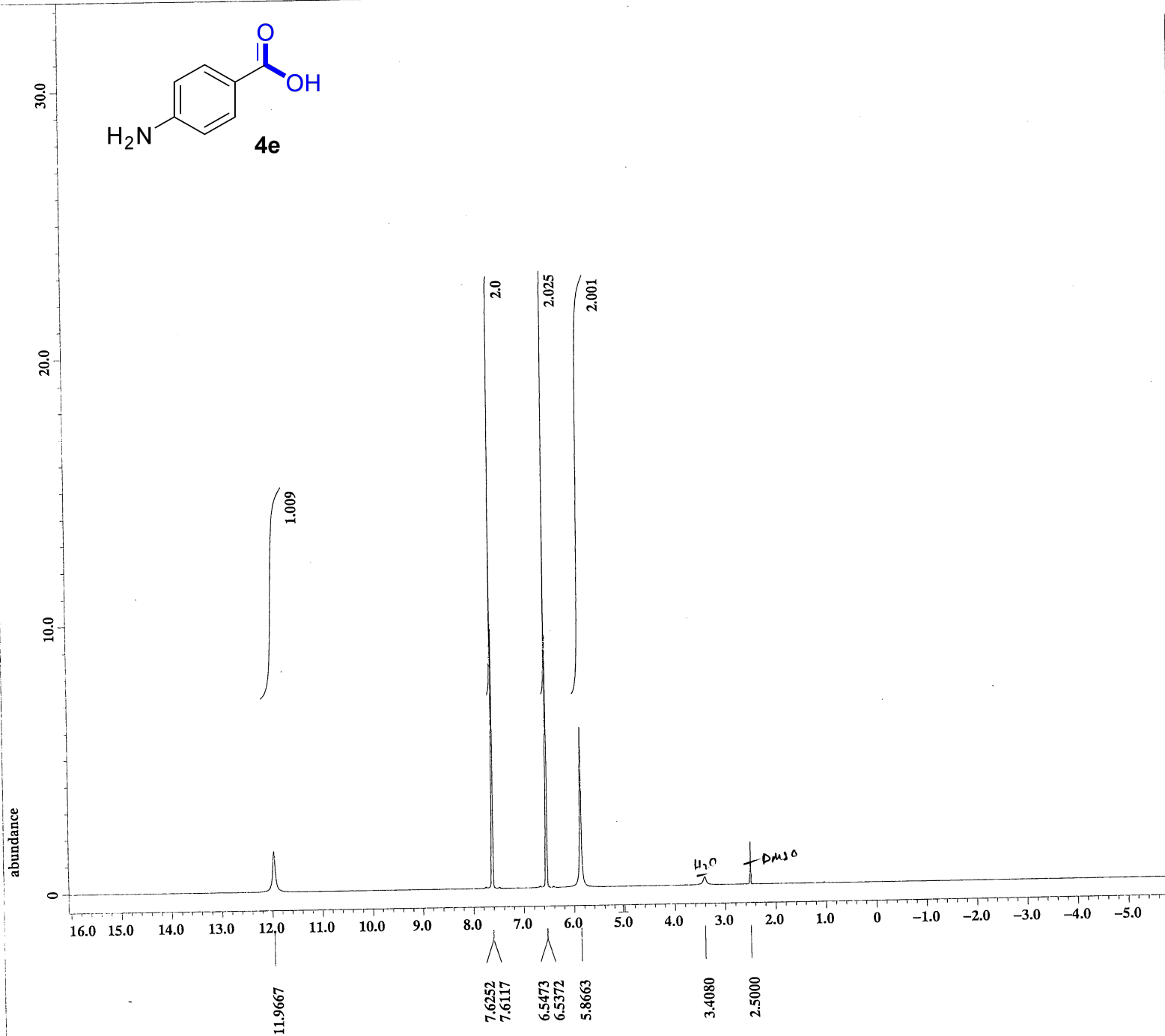
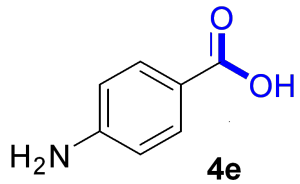
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sexp : 2.0 [Hz] : 0.0 [s]
 trapezoid3 : 0 [%] : 80 [%] : 100 [%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: Exp-R-165-17-1b-C-1.jdf

Filename = Exp-R-165-17-1b-C-2.j
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = Exp-R-165-17-1b-C
 Solvent = DMSO-D6
 Creation_time = 25-DEC-2018 20:15:31
 Revision_time = 25-DEC-2018 20:17:26
 Current_time = 25-DEC-2018 20:18:52

Comment = Exp-R-165-17-1b-C
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M])
 X_acq_duration = 0.69206016 [s]
 X_domain = 13C
 X_freq = 150.91343039 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109 [Hz]
 X_sweep = 47.34848485 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 56
 Total_scans = 56

X_90_width = 12.7 [us]
 X_acq_time = 0.69206016 [s]
 X_angle = 30 [deg]
 X_atn = 7.5 [dB]
 X_pulse = 4.23333333 [us]
 Irr_atn_dec = 18.62 [dB]
 Irr_atn_noe = 18.62 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.69206016 [s]
 Temp_get = 20.8 [dC]



X : parts per Million : 1H

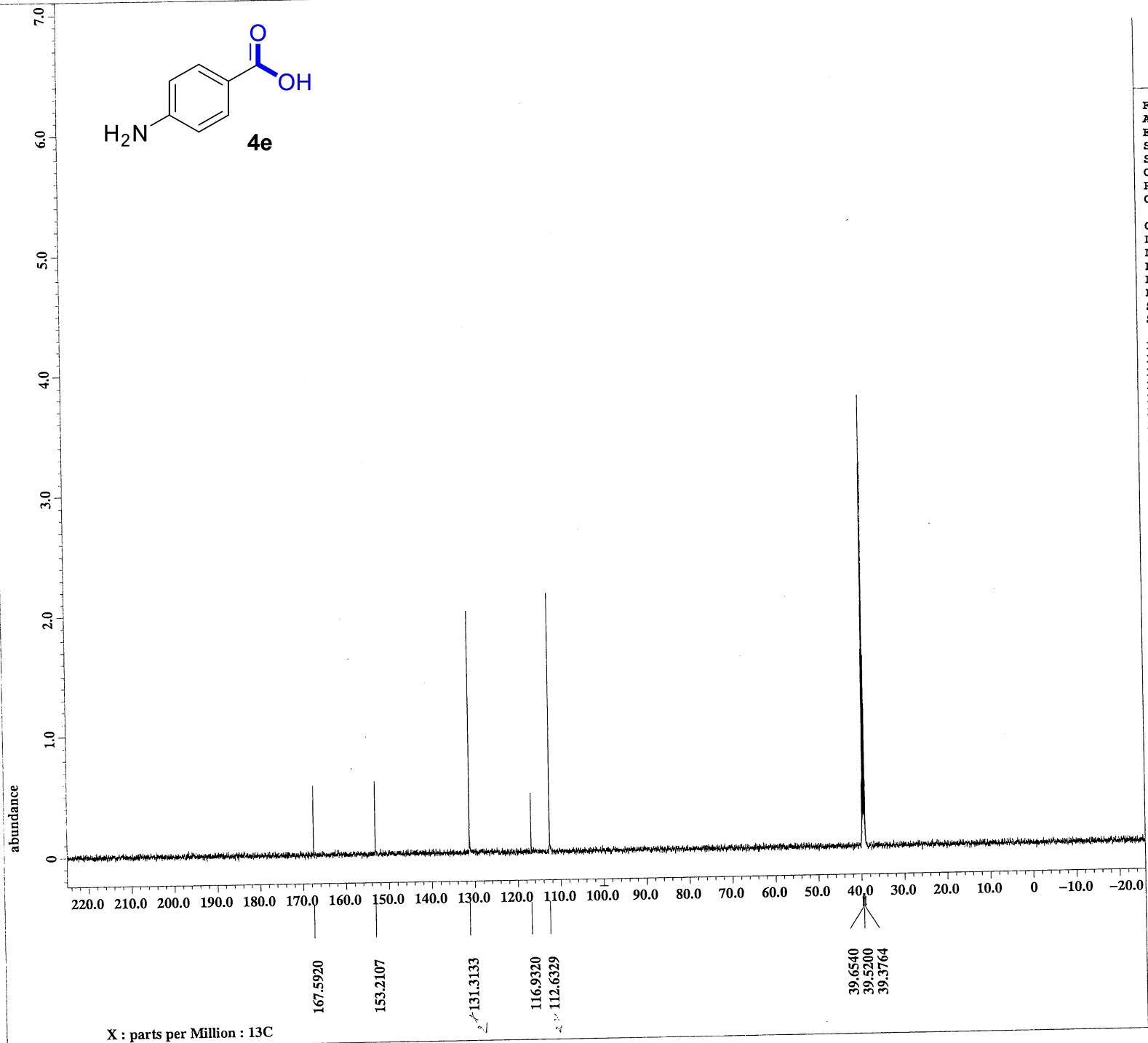
```

Filename      = Exp-R-124-17a-P-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-17a-P
Solvent      = DMSO-D6
Creation_time = 26-SEP-2018 16:31:17
Revision_time = 26-SEP-2018 16:39:57
Current_time  = 26-SEP-2018 16:39:59

Content      = Exp-R-124-17a-P
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 1.00917917[Hz]
X_sweep        = 16.53439153[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 12.68[us]
X_acq_time    = 0.99090432[s]
X_angle       = 45[deg]
X_atn         = 3.4[db]
X_pulse       = 6.34[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 44
Relaxation_delay = 5[s]
Repetition_time = 5.99090432[s]
Temp_get      = 21.1[dc]
  
```

```

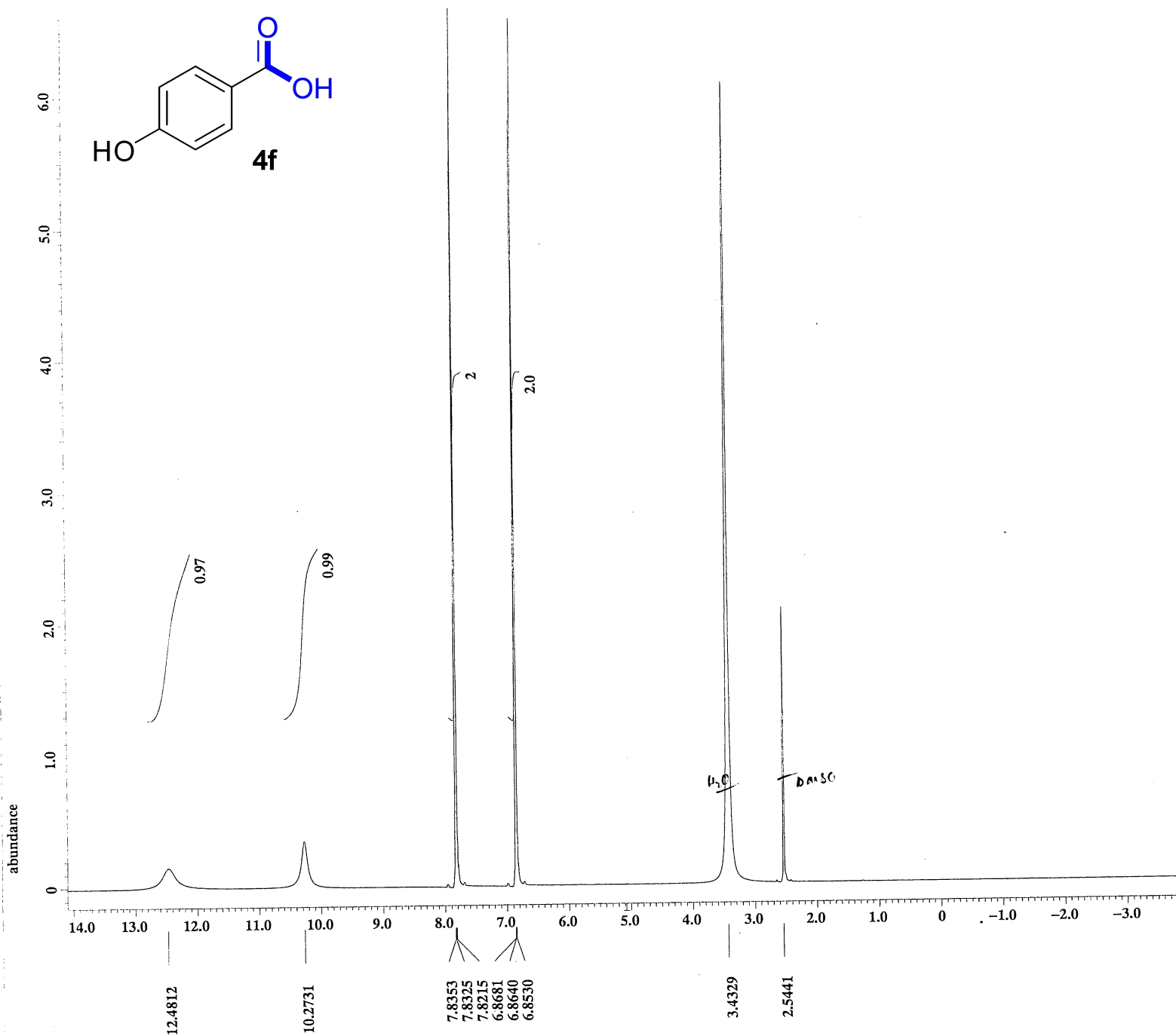
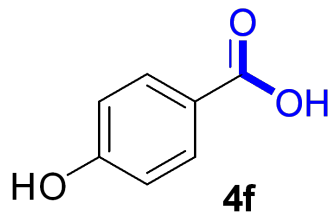
Filename      = Exp-R-124-17a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-17a-C
Solvent      = DMSO-D6
Creation_time = 26-SEP-2018 16:34:14
Revision_time = 26-SEP-2018 16:40:51
Current_time  = 26-SEP-2018 16:41:08

Content      = Exp-R-124-17a-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 40
Total_scans    = 40

X_90_width    = 12[us]
X_acq_time    = 0.69206016[s]
X_angle       = 30[deg]
X_atn         = 7.5[dB]
X_pulse       = 4[us]
Irr_atn_dec   = 18.95[dB]
Irr_atn_noe   = 18.95[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 2.5[s]
Recvr_gain    = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get      = 21.4[dC]

```



X : parts per Million : 1H

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

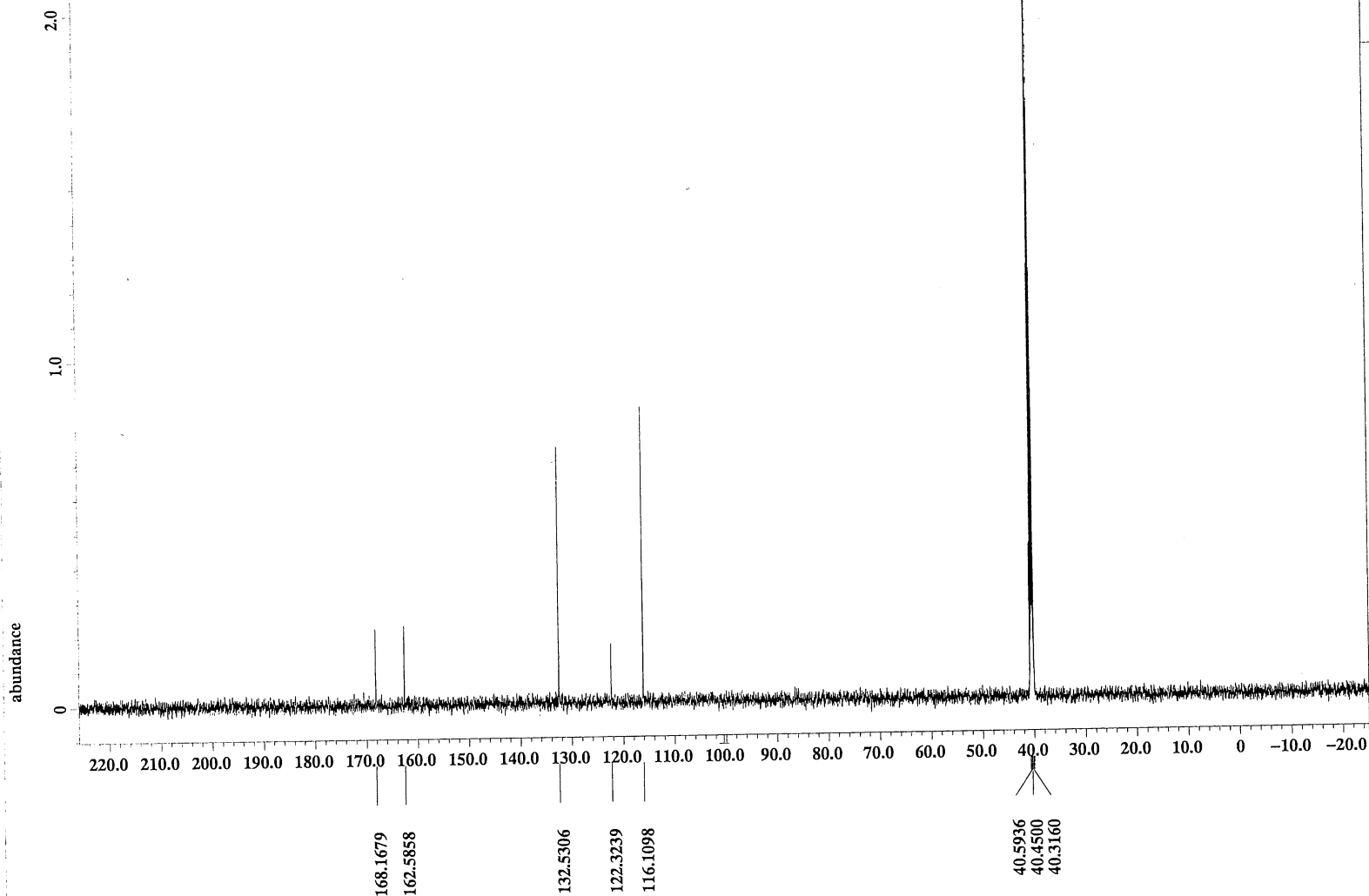
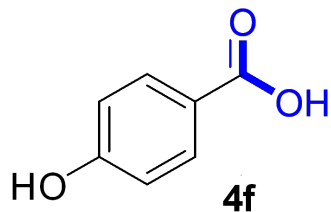
Derived from: Exp-AB-R-184-6-H-5.jdf

Filename = Exp-AB-R-184-6-H-10.j
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-AB-R-184-6-H
 Solvent = DMSO-D6
 Creation_time = 31-AUG-2020 11:25:51
 Revision_time = 31-AUG-2020 11:35:00
 Current_time = 31-AUG-2020 11:35:04

Comment = Exp-AB-R-184-6-H
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 1.21110528[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.82569205[Hz]
 X_sweep = 13.52813853[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17[us]
 X_acq_time = 1.21110528[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.585[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 5[s]
 Repetition_time = 6.21110528[s]
 Temp_get = 21.4[dc]



X : parts per Million : 13C

----- 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

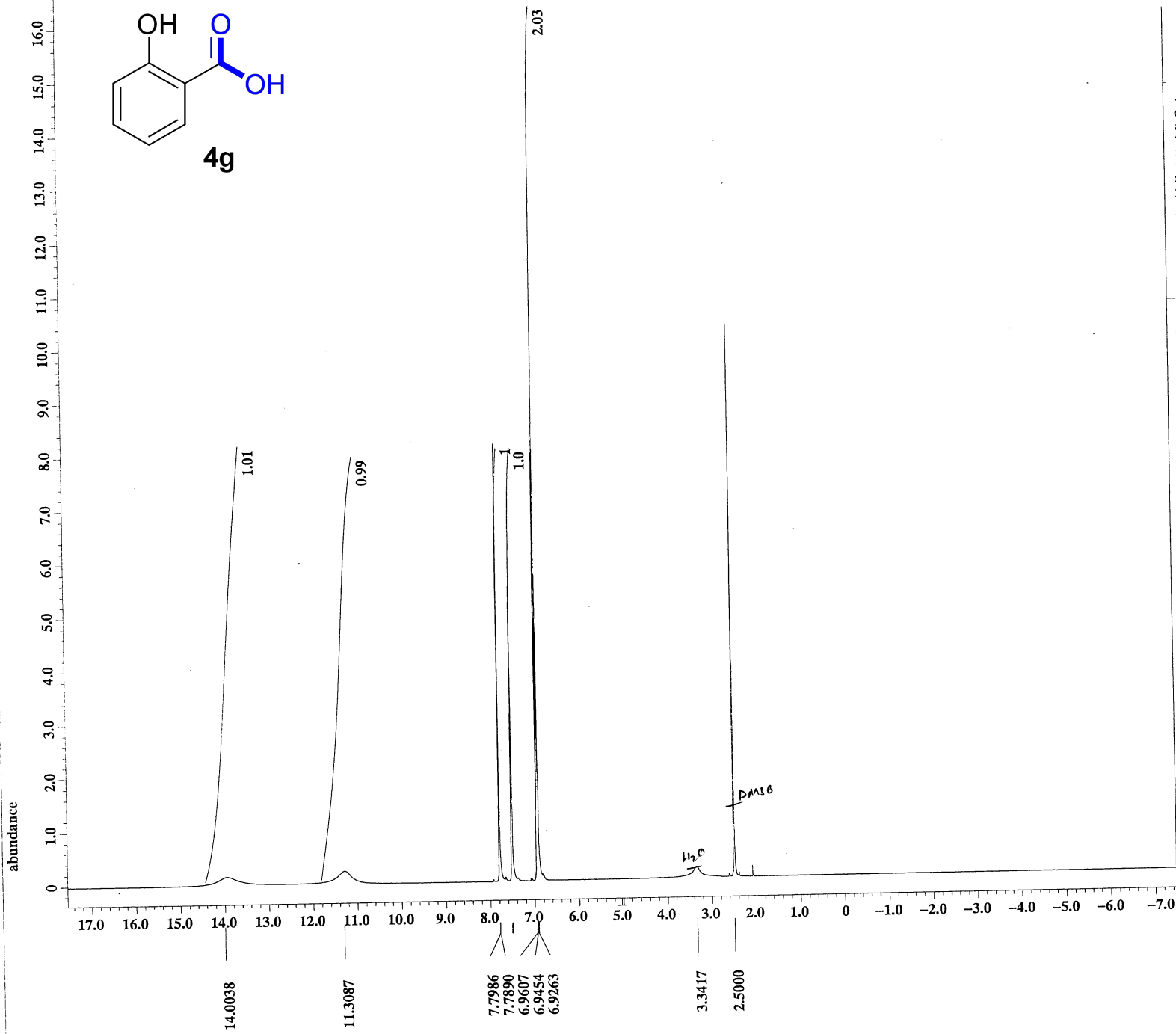
Derived from: Exp-AB-R-184-6-C-1.jdf

Filename = Exp-AB-R-184-6-C-3.jd
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = Exp-AB-R-184-6-C
 Solvent = DMSO-D6
 Creation_time = 31-AUG-2020 11:23:14
 Revision_time = 31-AUG-2020 11:30:45
 Current_time = 31-AUG-2020 11:30:55

Comment = Exp-AB-R-184-6-C
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.69206016[s]
 X_domain = 13C
 X_freq = 150.91343039[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109[Hz]
 X_sweep = 47.34848485[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 55
 Total_scans = 55

X_90_width = 12.3[us]
 X_acq_time = 0.69206016[s]
 X_angle = 30[deg]
 X_atn = 7.5[dB]
 X_pulse = 4.1[us]
 Irr_atn_dec = 18.62[dB]
 Irr_atn_noe = 18.62[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 60
 Relaxation_delay = 2[s]
 Repetition_time = 2.69206016[s]
 Temp_get = 21.8[dc]



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

Derived from: Exp-R-184-4-P-1.jdf

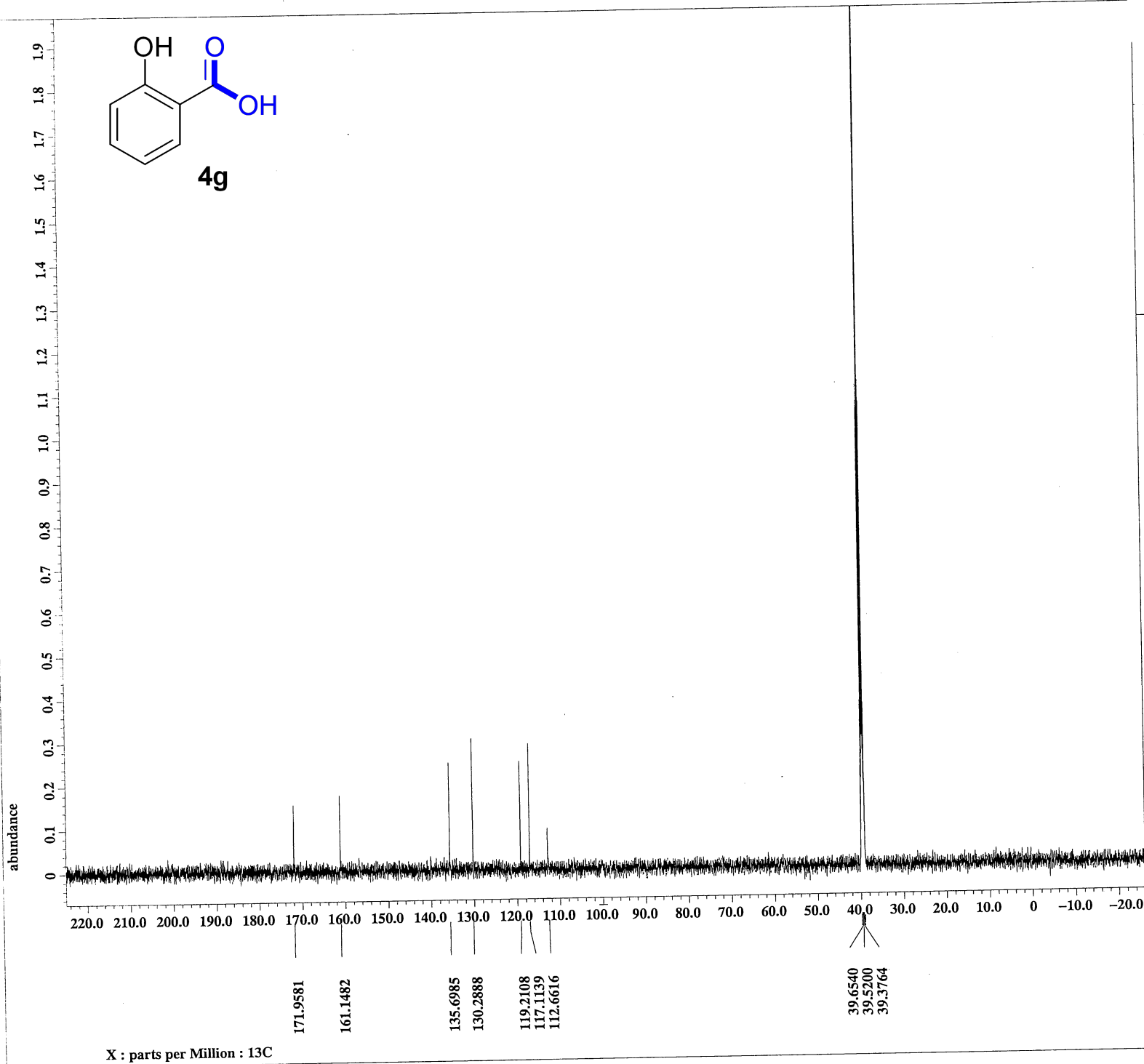
Filename = Exp-R-184-4-P-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-184-4-P
 Solvent = DMSO-D6
 Creation_time = 18-APR-2019 16:31:12
 Revision_time = 18-APR-2019 16:39:25
 Current_time = 18-APR-2019 16:39:40

Comment = Exp-R-184-4-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.87293952[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.14555473[Hz]
 X_sweep = 18.76876877[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17[us]
 X_acq_time = 0.87293952[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.585[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 56
 Relaxation_delay = 5[s]
 Repetition_time = 5.87293952[s]
 Temp_get = 20.6[dc]

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: Exp-R-184-4-C-1.jdf

```

Filename      = Exp-R-184-4-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-184-4-C
Solvent      = DMSO-D6
Creation_time = 18-APR-2019 16:35:36
Revision_time = 18-APR-2019 16:41:11
Current_time  = 18-APR-2019 16:41:16

```

```

Comment      = Exp-R-184-4-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

```

```

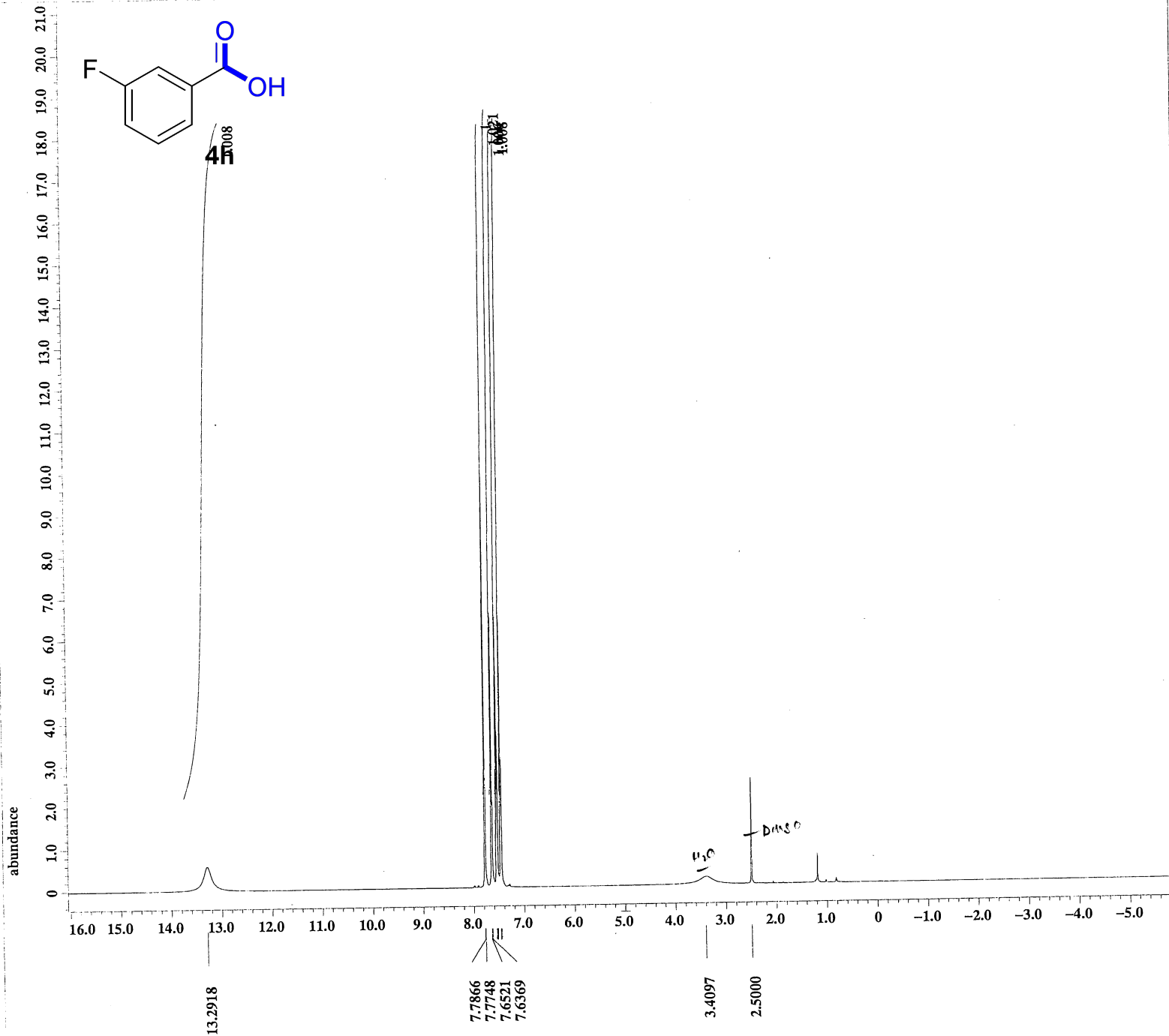
Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 82
Total_scans    = 82

```

```

X_90_width    = 12.7[us]
X_acq_time     = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 7.5[db]
X_pulse        = 4.23333333[us]
Irr_atn_dec    = 18.62[db]
Irr_atn_noe    = 18.62[db]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2[s]
Recvr_gain     = 60
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get       = 21.7[dc]

```



```

Filename      = Exp-R-124-20b-P-5.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-20b-P
Solvent      = DMSO-D6
Creation_time = 14-AUG-2018 16:32:06
Revision_time = 14-AUG-2018 17:04:57
Current_time  = 14-AUG-2018 17:05:01
  
```

```

Content       = Exp-R-124-20b-P
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 600
Spectrometer  = DELTA2_NMR
  
```

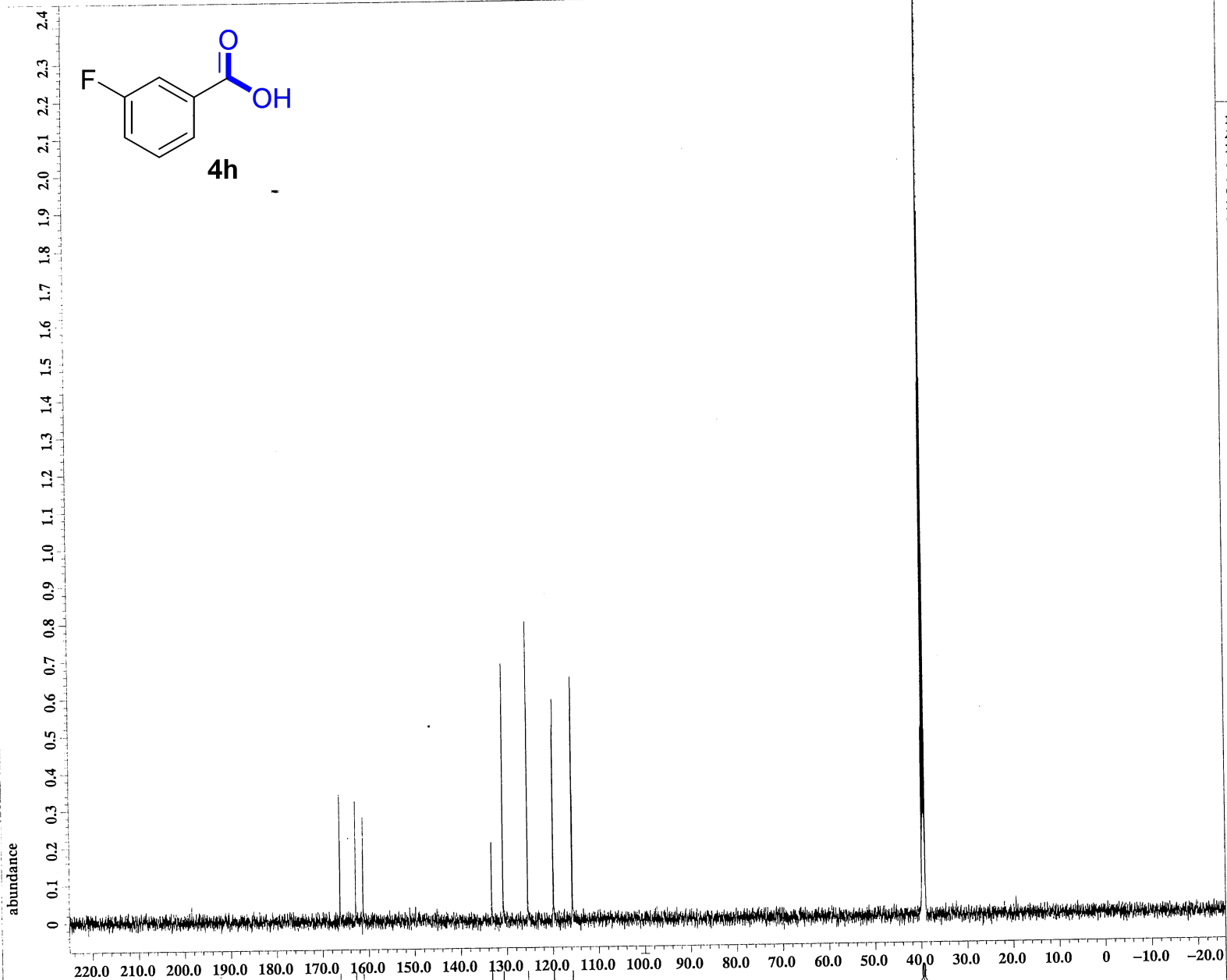
```

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 1.00917917[Hz]
X_sweep        = 16.53439153[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8
  
```

```

X_90_width    = 12.68[us]
X_acq_time     = 0.99090432[s]
X_angle        = 45[deg]
X_atn          = 3.4[db]
X_pulse        = 6.34[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 46
Relaxation_delay = 5[s]
Repetition_time = 5.99090432[s]
Temp_get       = 22.2[dc]
  
```

X : parts per Million : 1H



```

Filename      = Exp-R-124-20b-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-20b-C
Solvent      = DMSO-D6
Creation_time = 14-AUG-2018 16:36:26
Revision_time = 14-AUG-2018 17:06:36
Current_time  = 14-AUG-2018 17:07:02

Content      = Exp-R-124-20b-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

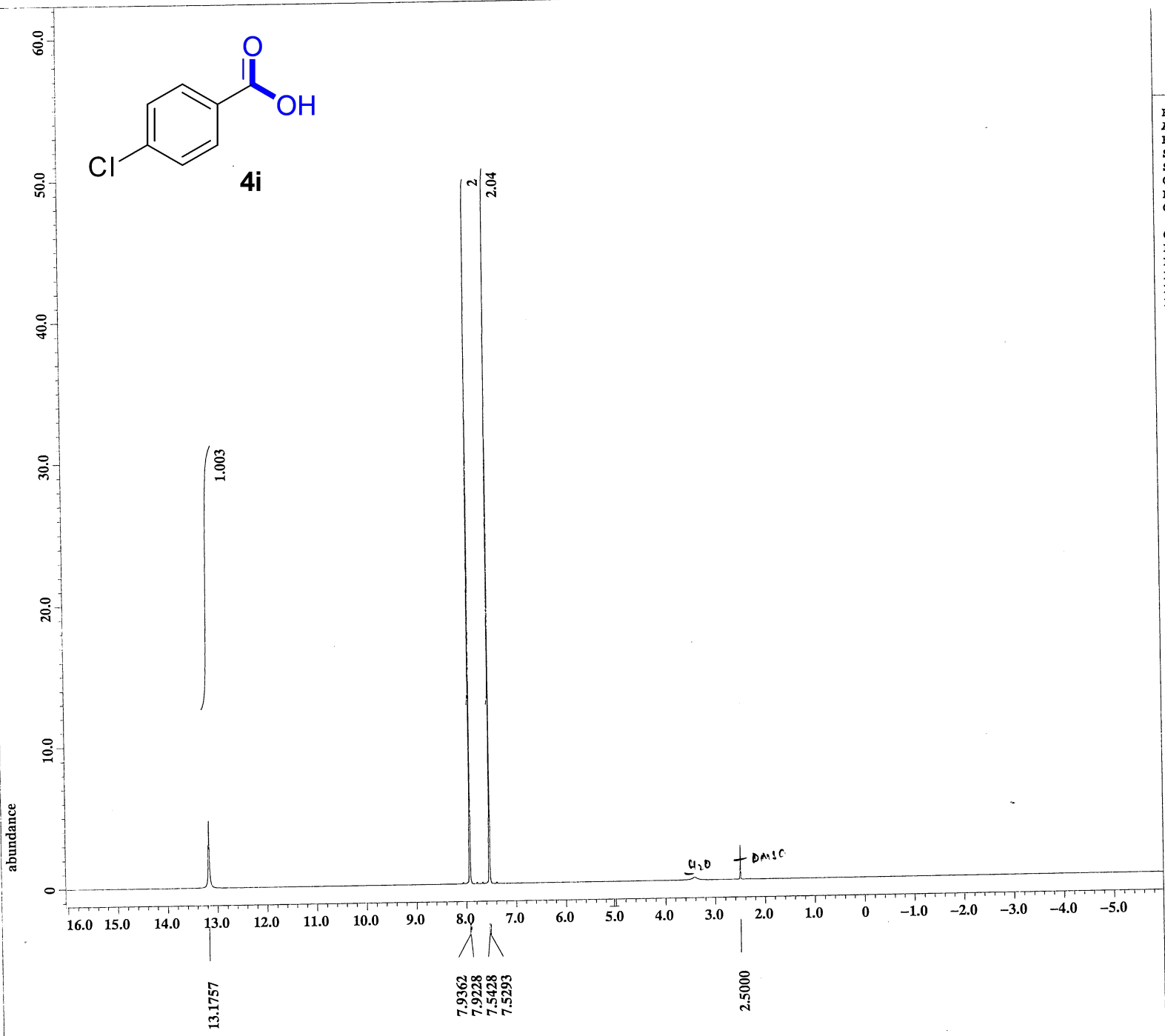
Field_strength = 14.09636928 [T] (600[M]
X_acq_duration = 0.69206016 [s]
X_domain       = 13C
X_freq         = 150.91343039 [MHZ]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109 [Hz]
X_sweep        = 47.34848485 [kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046 [MHZ]
Irr_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 66
Total_scans    = 66

X_90_width     = 12 [us]
X_acq_time     = 0.69206016 [s]
X_angle        = 30 [deg]
X_atn          = 7.5 [dB]
X_pulse        = 4 [us]
Irr_atn_dec    = 18.95 [dB]
Irr_atn_noe    = 18.95 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2.5 [s]
Recvr_gain     = 60
Relaxation_delay = 2.5 [s]
Repetition_time = 3.19206016 [s]
Temp_get       = 22.5 [dC]
  
```

166.2516
 162.8334
 161.2152
 133.2857
 130.8441
 130.7962
 125.4822
 119.9576
 119.8235
 115.8692
 115.7160

39.6636
 39.5200
 39.3860

X : parts per Million : 13C



X : parts per Million : 1H

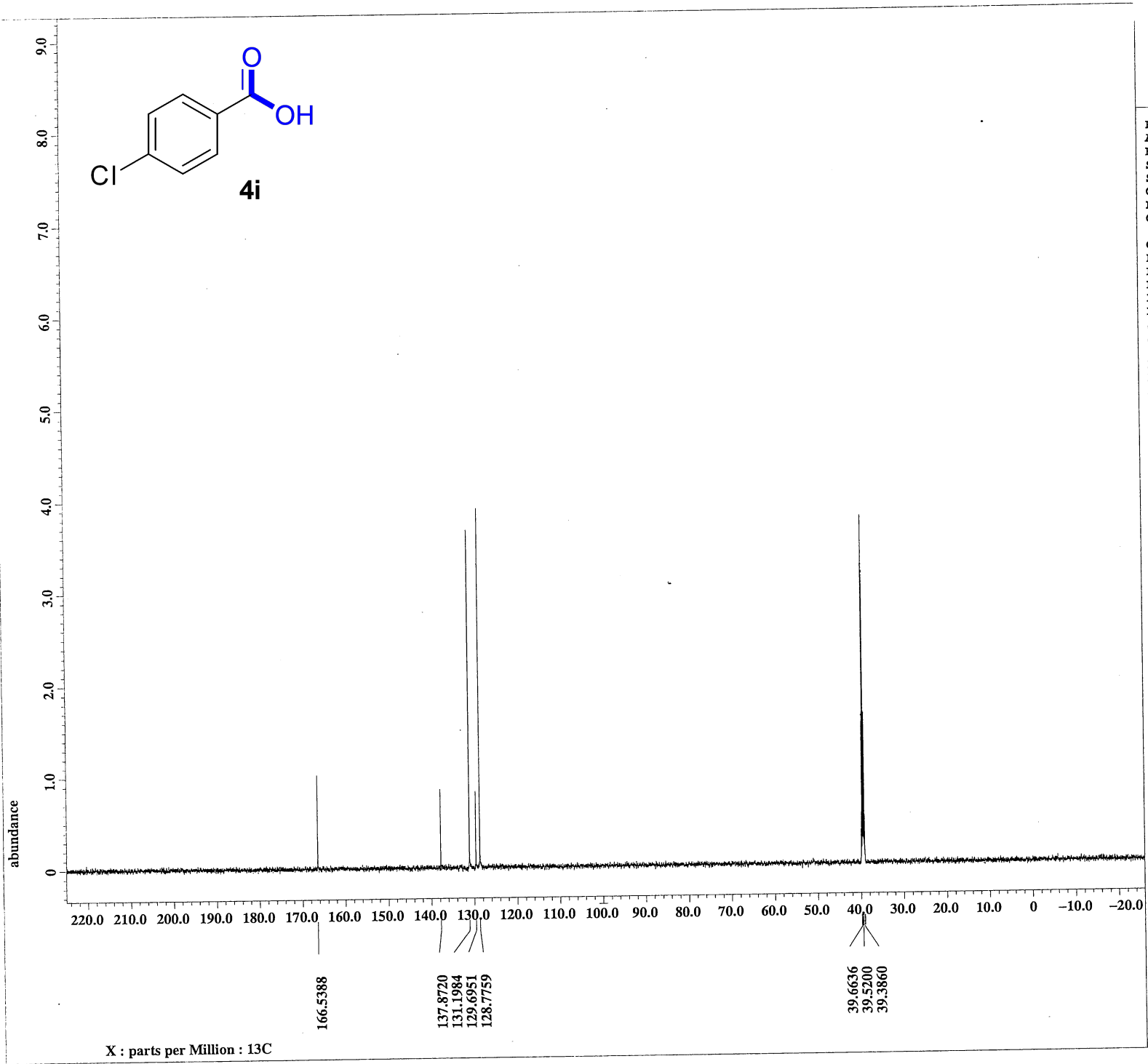
```

Filename      = Exp-R-124-p-Cl-benzoi
Author        = delta
Experiment    = single_pulse.ex2
Sample_id     = Exp-R-124-p-Cl-benzoi
Solvent       = DMSO-D6
Creation_time = 21-SEP-2018 19:34:47
Revision_time = 21-SEP-2018 19:42:54
Current_time  = 21-SEP-2018 19:42:56

Content       = Exp-R-124-p-Cl-benzoi
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain      = 1H
X_freq       = 600.1723046[MHz]
X_offset     = 5[ppm]
X_points     = 16384
X_prescans   = 1
X_resolution = 1.00917917[Hz]
X_sweep      = 16.53439153[kHz]
Irr_domain   = 1H
Irr_freq     = 600.1723046[MHz]
Irr_offset   = 5[ppm]
Tri_domain   = 1H
Tri_freq     = 600.1723046[MHz]
Tri_offset   = 5[ppm]
Clipped      = FALSE
Mod_return   = 1
Scans        = 8
Total_scans  = 8

X_90_width   = 12.68[us]
X_acq_time   = 0.99090432[s]
X_angle      = 45[deg]
X_atn        = 3.4[dB]
X_pulse      = 6.34[us]
Irr_mode     = Off
Tri_mode     = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain   = 44
Relaxation_delay = 5[s]
Repetition_time = 5.99090432[s]
Temp_get     = 21[degC]
  
```

```

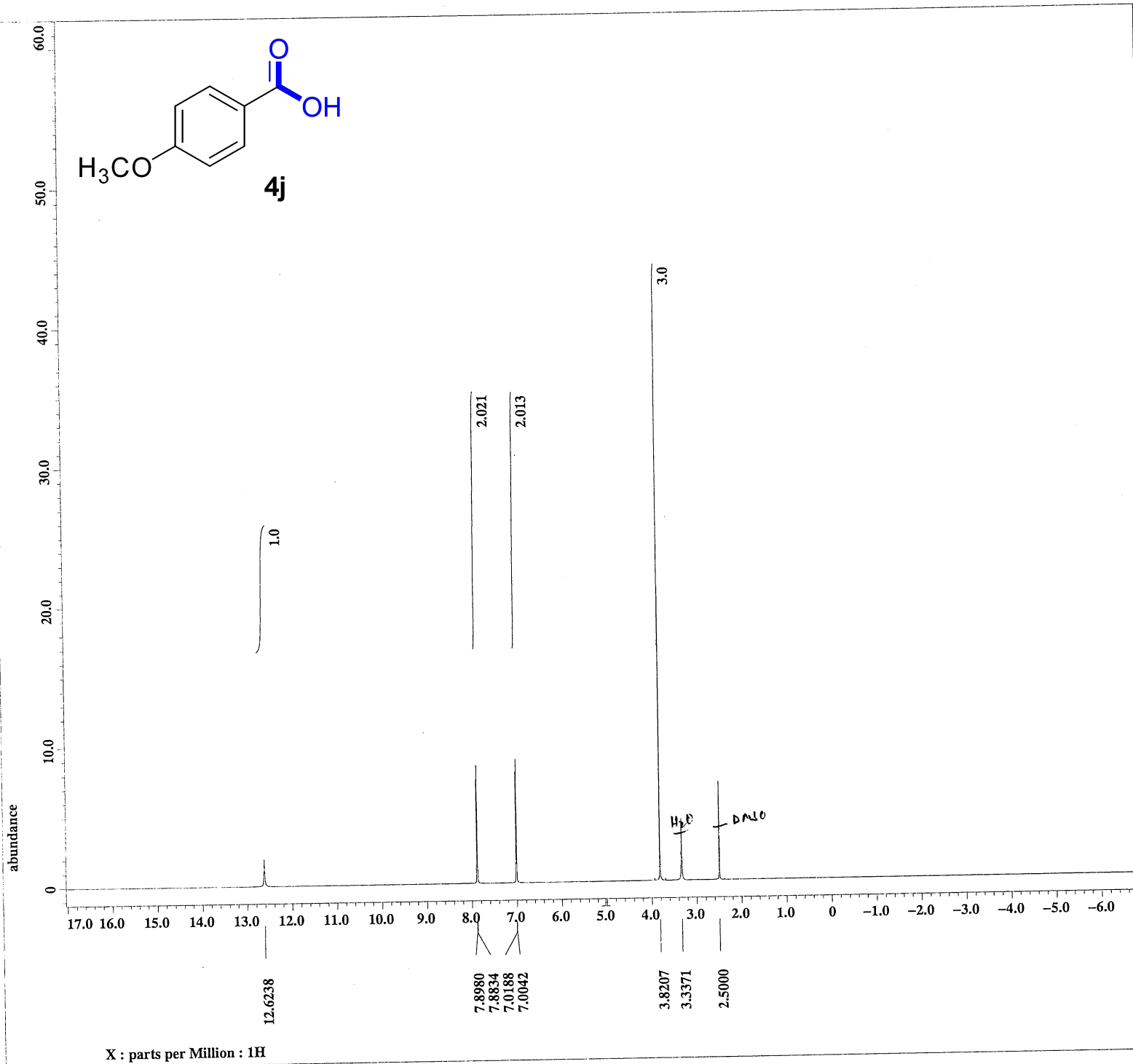
Filename      = Exp-R-124-p-Cl-benzoi
Author        = delta
Experiment    = single_pulse_dec
Sample_id     = Exp-R-124-p-Cl-benzoi
Solvent       = DMSO-D6
Creation_time = 21-SEP-2018 19:37:17
Revision_time = 21-SEP-2018 19:45:50
Current_time  = 21-SEP-2018 19:45:58

Content       = Exp-R-124-p-Cl-benzoi
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 32
Total_scans    = 32

X_90_width    = 12[us]
X_acq_time     = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 7.5[dB]
X_pulse        = 4[us]
Irr_atn_dec    = 18.95[dB]
Irr_atn_noe    = 18.95[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2.5[s]
Recvr_gain     = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get       = 21.4[dC]

```

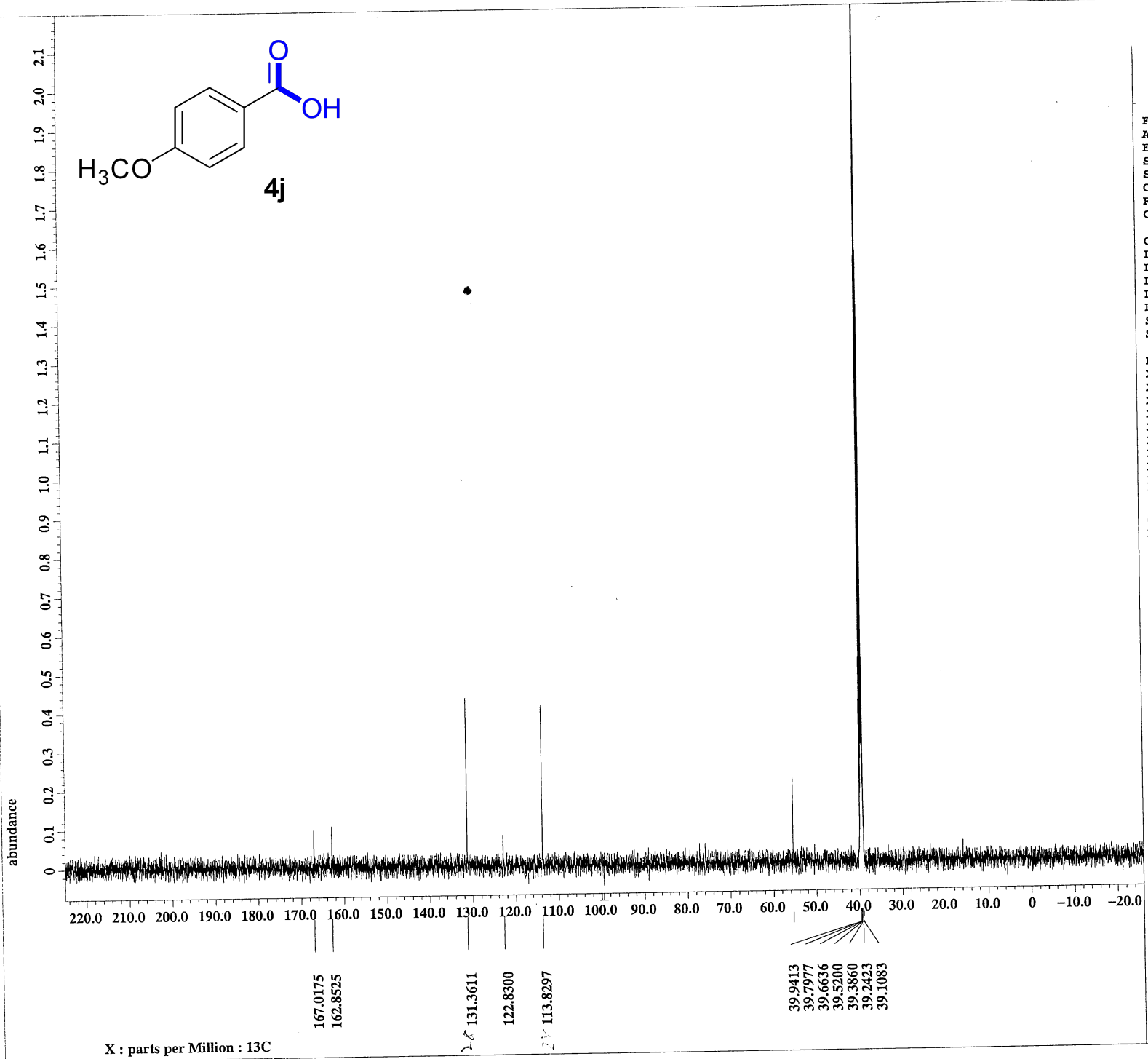


Filename = Exp-R-124-15a-P-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-124-15a-P
 Solvent = DMSO-D6
 Creation_time = 25-SEP-2018 19:29:00
 Revision_time = 25-SEP-2018 19:37:56
 Current_time = 25-SEP-2018 19:38:01

Content = Exp-R-124-15a-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.90963968[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.09933639[Hz]
 X_sweep = 18.01152738[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 12.68[us]
 X_acq_time = 0.90963968[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.34[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 54
 Relaxation_delay = 5[s]
 Repetition_time = 5.90963968[s]
 Temp_get = 21.4[degC]



```

Filename      = Exp-R-124-15a-C-5.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-15a-C
Solvent      = DMSO-D6
Creation_time = 25-SEP-2018 19:32:04
Revision_time = 25-SEP-2018 19:39:53
Current_time  = 25-SEP-2018 19:40:02

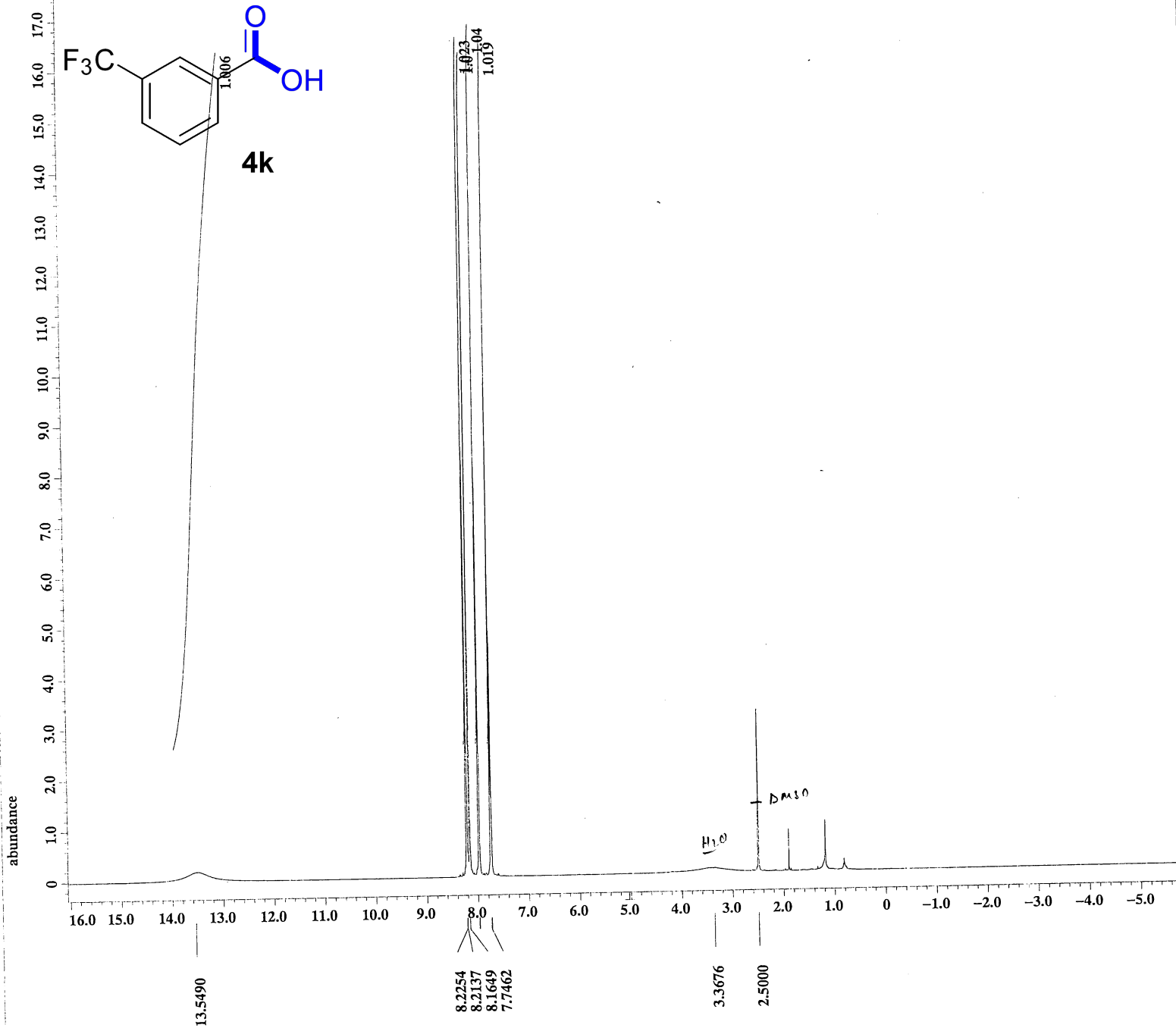
Content      = Exp-R-124-15a-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 42
Total_scans    = 42

X_90_width    = 12[us]
X_acq_time    = 0.69206016[s]
X_angle       = 30[deg]
X_atn         = 7.5[dB]
X_pulse       = 4[us]
Irr_atn_dec   = 18.95[dB]
Irr_atn_noe   = 18.95[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 2.5[s]
Recvr_gain    = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get      = 21.7[dC]

```

X : parts per Million : 13C



```

Filename      = Exp-R-124-22a-P-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-124-22a-P
Solvent      = DMSO-D6
Creation_time = 23-AUG-2018 18:27:10
Revision_time = 23-AUG-2018 18:32:23
Current_time  = 23-AUG-2018 18:32:26

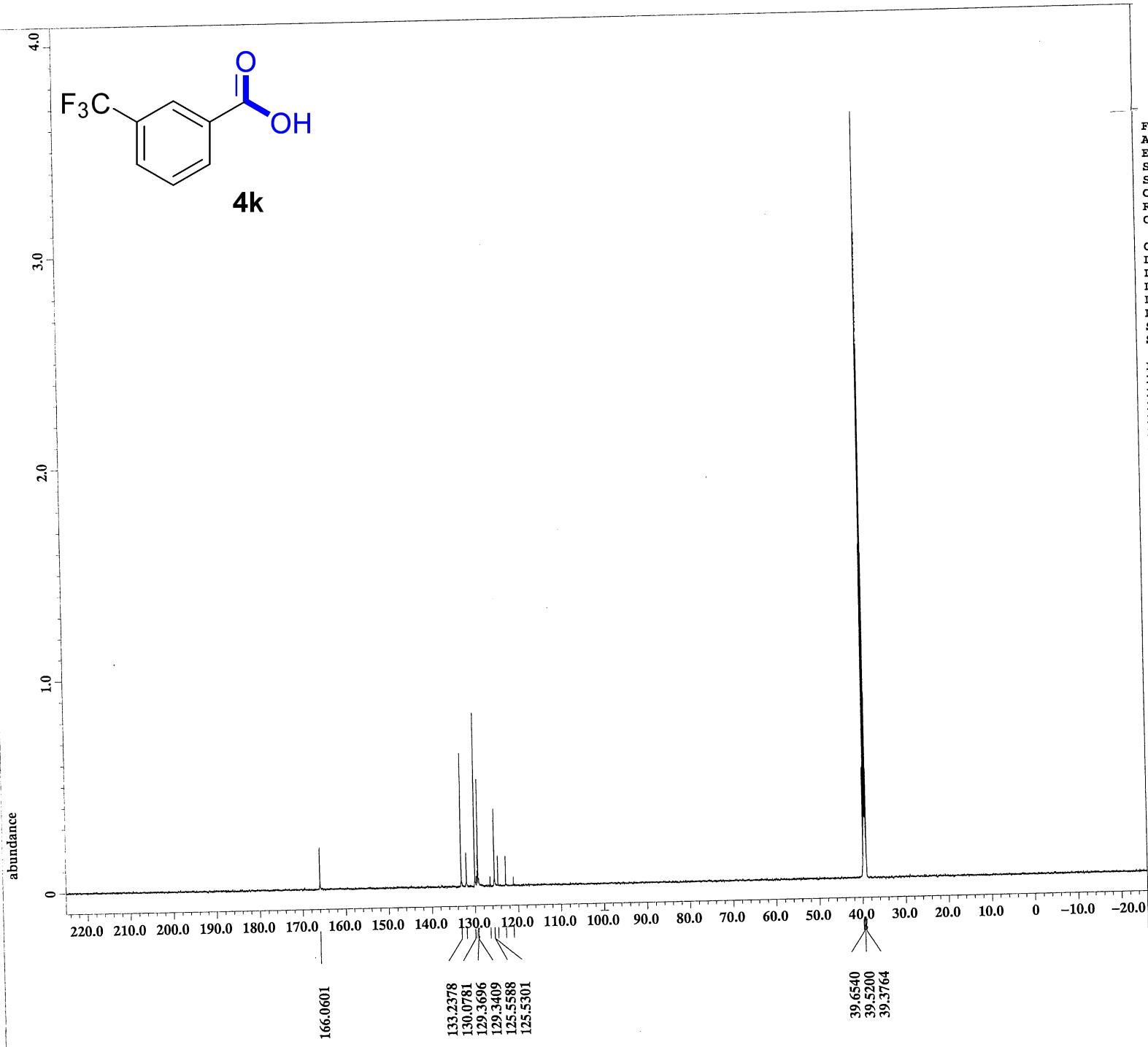
Content       = Exp-R-124-22a-P
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.99090432[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans    = 1
X_resolution   = 1.00917917[Hz]
X_sweep        = 16.53439153[kHz]
Irr_domain    = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain    = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 8
Total_scans   = 8

X_90_width    = 12.68[us]
X_acq_time    = 0.99090432[s]
X_angle       = 45[deg]
X_atn         = 3.4[dB]
X_pulse       = 6.34[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 48
Relaxation_delay = 5[s]
Repetition_time = 5.99090432[s]
Temp_get      = 21.5[dC]

```

X : parts per Million : 1H



```

Filename      = Exp-R-124-22a-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-124-22a-C
Solvent      = DMSO-D6
Creation_time = 23-AUG-2018 19:04:17
Revision_time = 23-AUG-2018 19:09:20
Current_time  = 23-AUG-2018 19:09:57

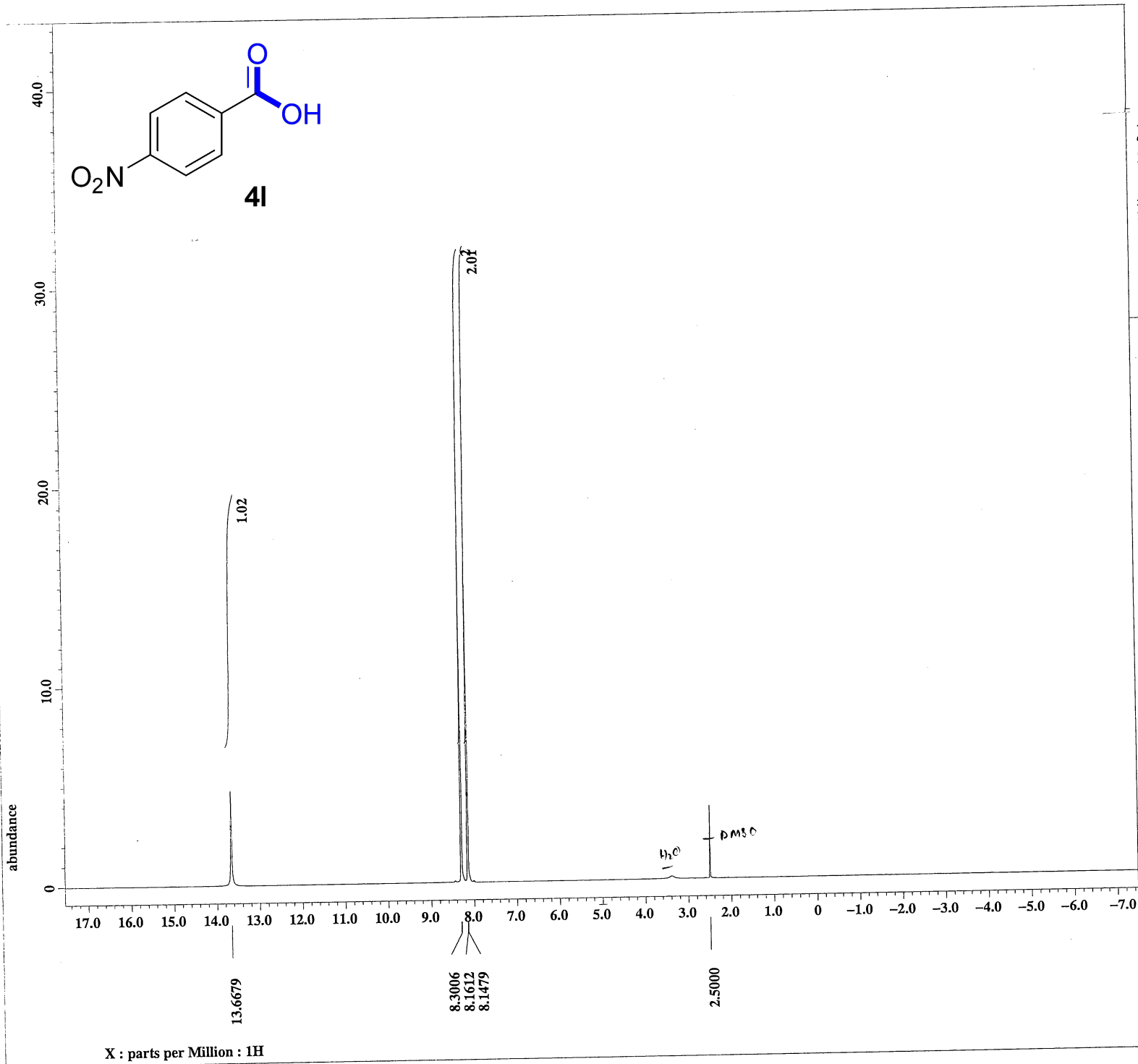
Content      = Exp-R-124-22a-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = TRUE
Mod_return     = 1
Scans          = 682
Total_scans    = 682

X_90_width    = 12[us]
X_acq_time     = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 7.5[dB]
X_pulse        = 4[us]
Irr_atn_dec    = 18.95[dB]
Irr_atn_noe    = 18.95[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2.5[s]
Recvr_gain     = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.19206016[s]
Temp_get       = 22[degC]

```

X : parts per Million : 13C



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

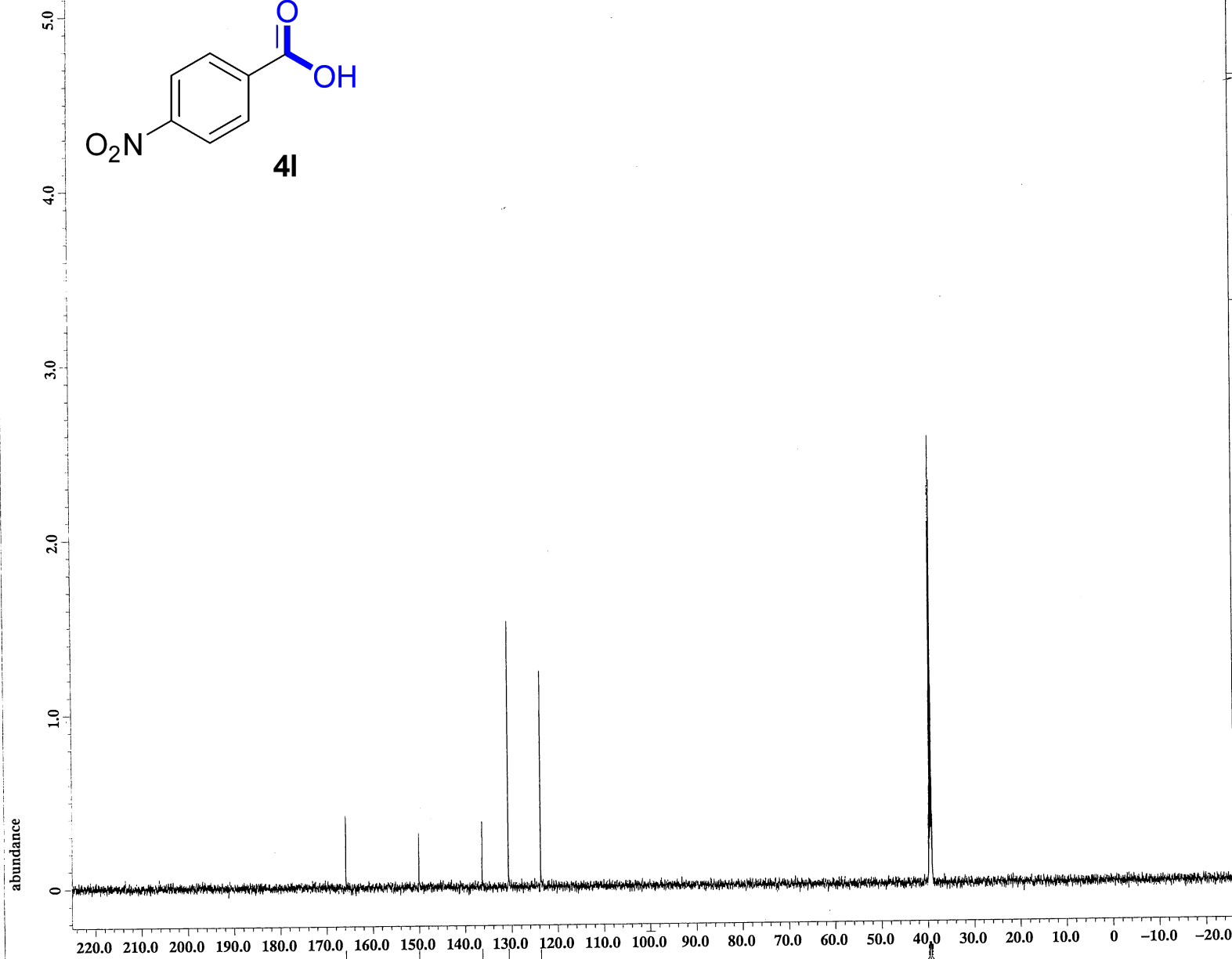
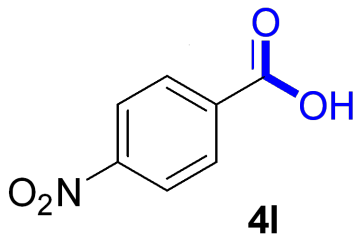
Derived from: Exp-R-184-1a-P-2.jdf

Filename = Exp-R-184-1a-P-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-184-1a-P
 Solvent = DMSO-D6
 Creation_time = 18-APR-2019 15:59:18
 Revision_time = 18-APR-2019 16:05:31
 Current_time = 18-APR-2019 16:05:35

Comment = Exp-R-184-1a-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.87293952[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.14555473[Hz]
 X_sweep = 18.76876877[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17[us]
 X_acq_time = 0.87293952[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.585[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 5[s]
 Repetition_time = 5.87293952[s]
 Temp_get = 20.9[dC]



----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sexp : 2.0[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: Exp-R-184-1a-C-2.jdf

```

Filename      = Exp-R-184-1a-C-4.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = Exp-R-184-1a-C
Solvent      = DMSO-D6
Creation_time = 18-APR-2019 16:01:35
Revision_time = 18-APR-2019 16:14:51
Current_time = 18-APR-2019 16:14:59

Comment      = Exp-R-184-1a-C
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 35
Total_scans    = 35

X_90_width    = 12.7[us]
X_acq_time     = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 7.5[db]
X_pulse        = 4.23333333[us]
Irr_atn_dec    = 18.62[db]
Irr_atn_noe    = 18.62[db]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2[s]
Recvr_gain     = 60
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get       = 21.6[dc]
  
```

X : parts per Million : 13C

```

----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: Exp-R-124-11-1-P-1.jdf

```

```

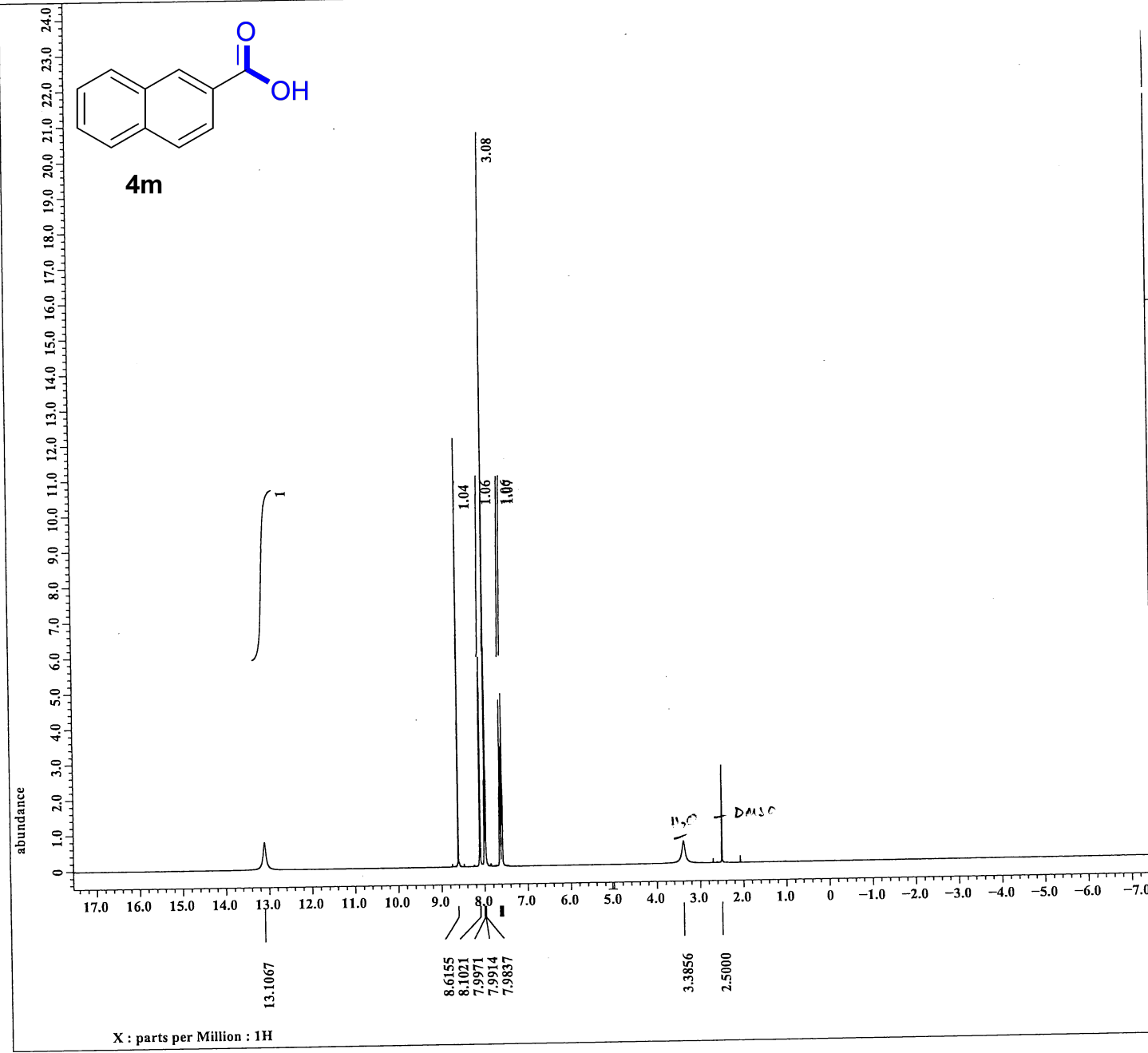
Filename      = Exp-R-124-11-1-P-4.jd
Author        = delta
Experiment    = single_pulse.ex2
Sample_id     = Exp-R-124-11-1-P
Solvent       = DMSO-D6
Creation_time = 12-DEC-2018 17:45:52
Revision_time = 12-DEC-2018 17:53:43
Current_time  = 12-DEC-2018 17:54:23

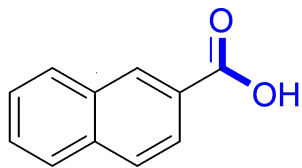
Comment       = Exp-R-124-11-1-P
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 600
Spectrometer  = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.87293952[s]
X_domain       = 1H
X_freq        = 600.1723046 [MHz]
X_offset      = 5 [ppm]
X_points      = 16384
X_prescans    = 1
X_resolution  = 1.14555473 [Hz]
X_sweep       = 18.76876877 [kHz]
Irr_domain    = 1H
Irr_freq      = 600.1723046 [MHz]
Irr_offset    = 5 [ppm]
Tri_domain    = 1H
Tri_freq      = 600.1723046 [MHz]
Tri_offset    = 5 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 8
Total_scans   = 8

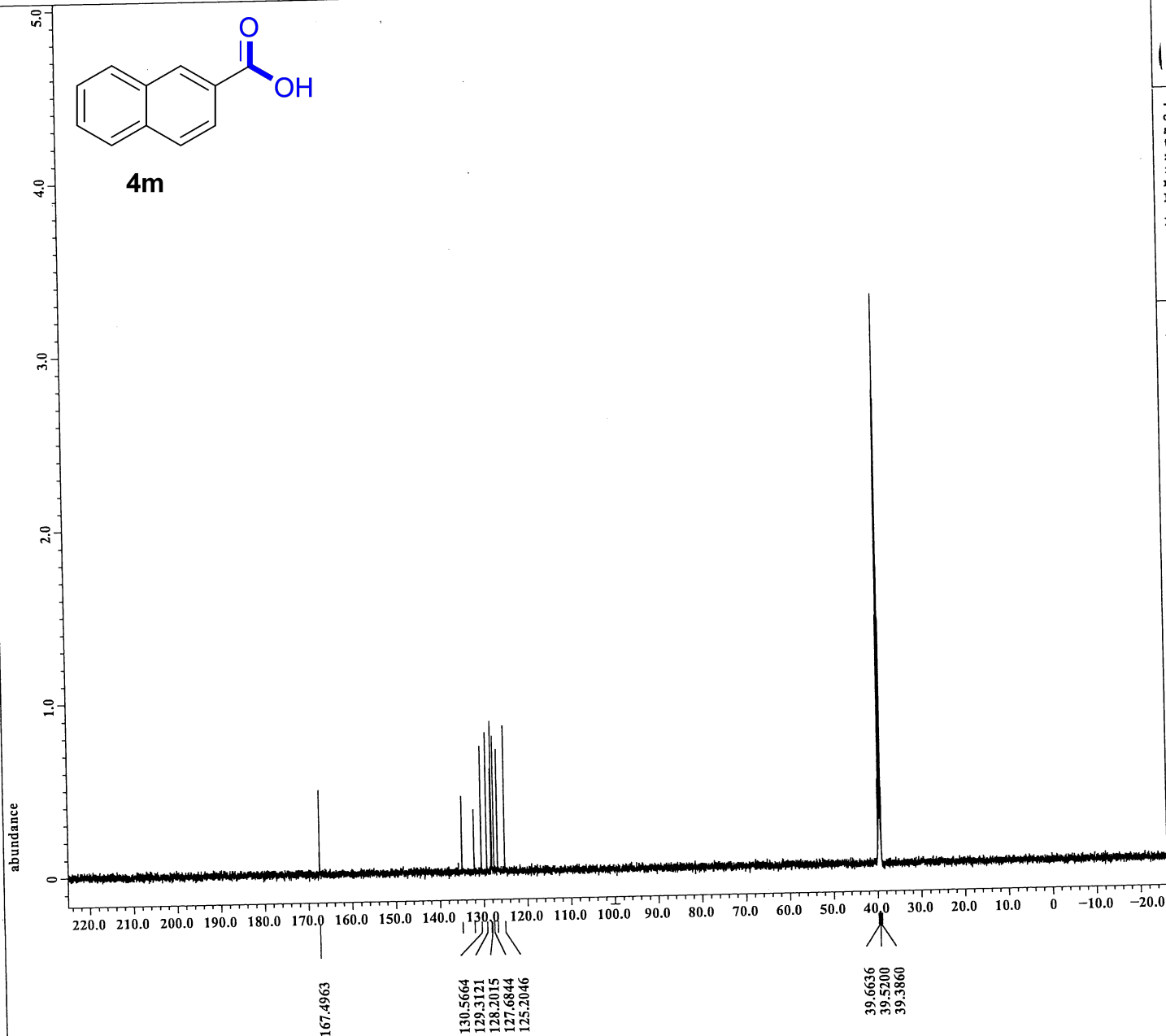
X_90_width    = 13.17 [us]
X_acq_time     = 0.87293952 [s]
X_angle       = 45 [deg]
X_atn         = 3.4 [dB]
X_atn         = 6.585 [us]
X_pulse       = Off
Irr_mode      = Off
Tri_mode      = Off
Dante_preset  = FALSE
Initial_wait  = 1 [s]
Recvr_gain    = 44
Relaxation_delay = 5 [s]
Repetition_time = 5.87293952 [s]
Temp_get      = 20.9 [dc]

```





4m



X : parts per Million : 13C

---- 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

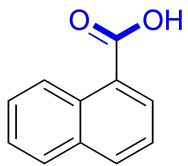
Derived from: Exp-R-124-11-1-C-1.jdf

Filename = Exp-R-124-11-1-C-3.jd
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = Exp-R-124-11-1-C
 Solvent = DMSO-D6
 Creation_time = 12-DEC-2018 17:49:11
 Revision_time = 12-DEC-2018 17:55:43
 Current_time = 12-DEC-2018 17:56:13

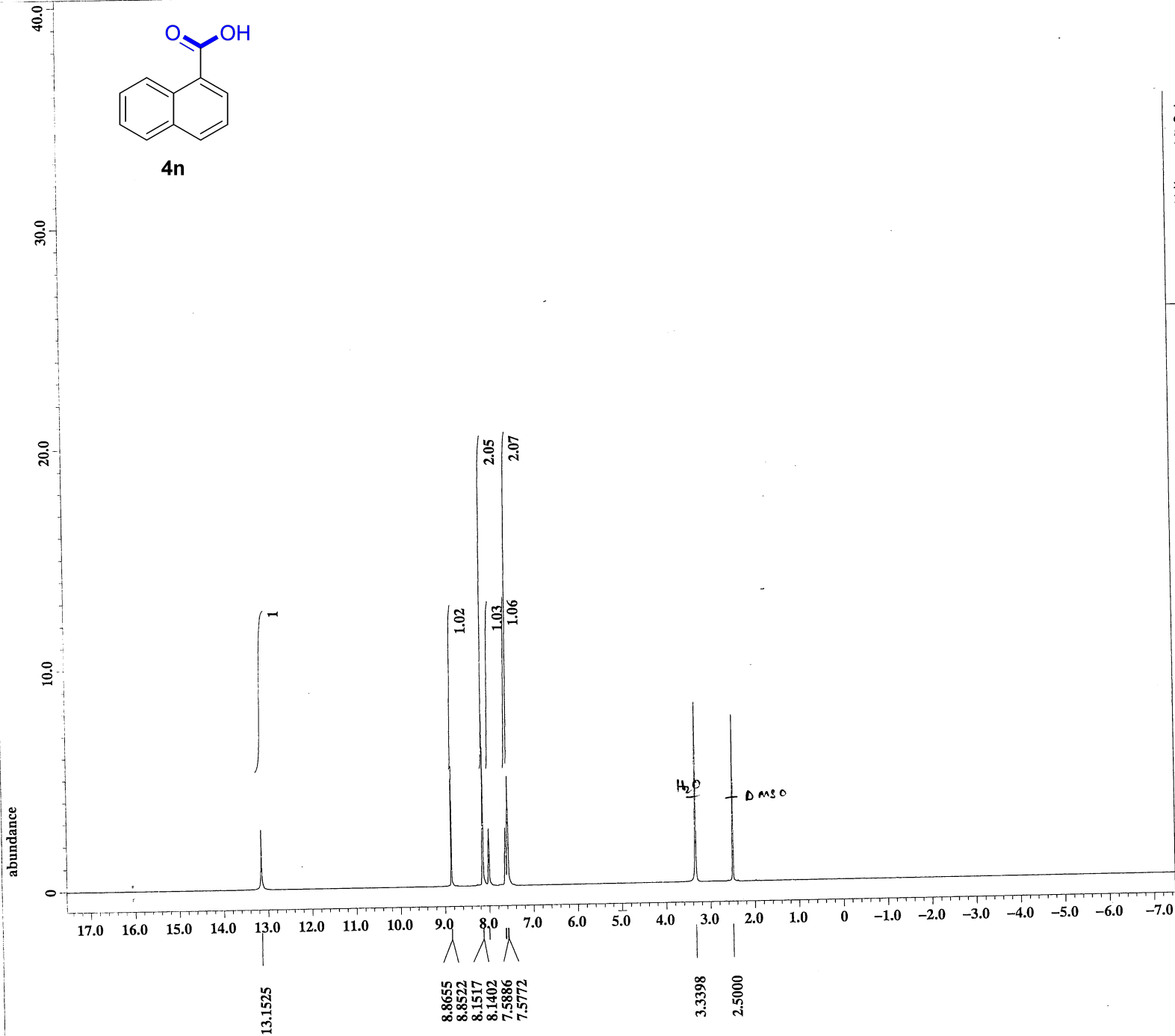
Comment = Exp-R-124-11-1-C
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M])
 X_acq_duration = 0.69206016 [s]
 X_domain = 13C
 X_freq = 150.91343039 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109 [Hz]
 X_sweep = 47.34848485 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 58
 Total_scans = 58

X_90_width = 12.7 [us]
 X_acq_time = 0.69206016 [s]
 X_angle = 30 [deg]
 X_atn = 7.5 [dB]
 X_pulse = 4.23333333 [us]
 Irr_atn_dec = 18.62 [dB]
 Irr_atn_noe = 18.62 [dB]
 Irr_noise = WAITZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.69206016 [s]
 Temp_get = 21.7 [dC]



4n



X : parts per Million : 1H

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

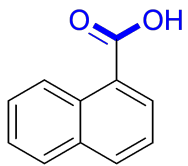
Derived from: Exp-R-184-6-P-1.jdf

Filename = Exp-R-184-6-P-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-184-6-P
 Solvent = DMSO-D6
 Creation_time = 18-APR-2019 16:52:20
 Revision_time = 18-APR-2019 16:59:24
 Current_time = 18-APR-2019 16:59:28

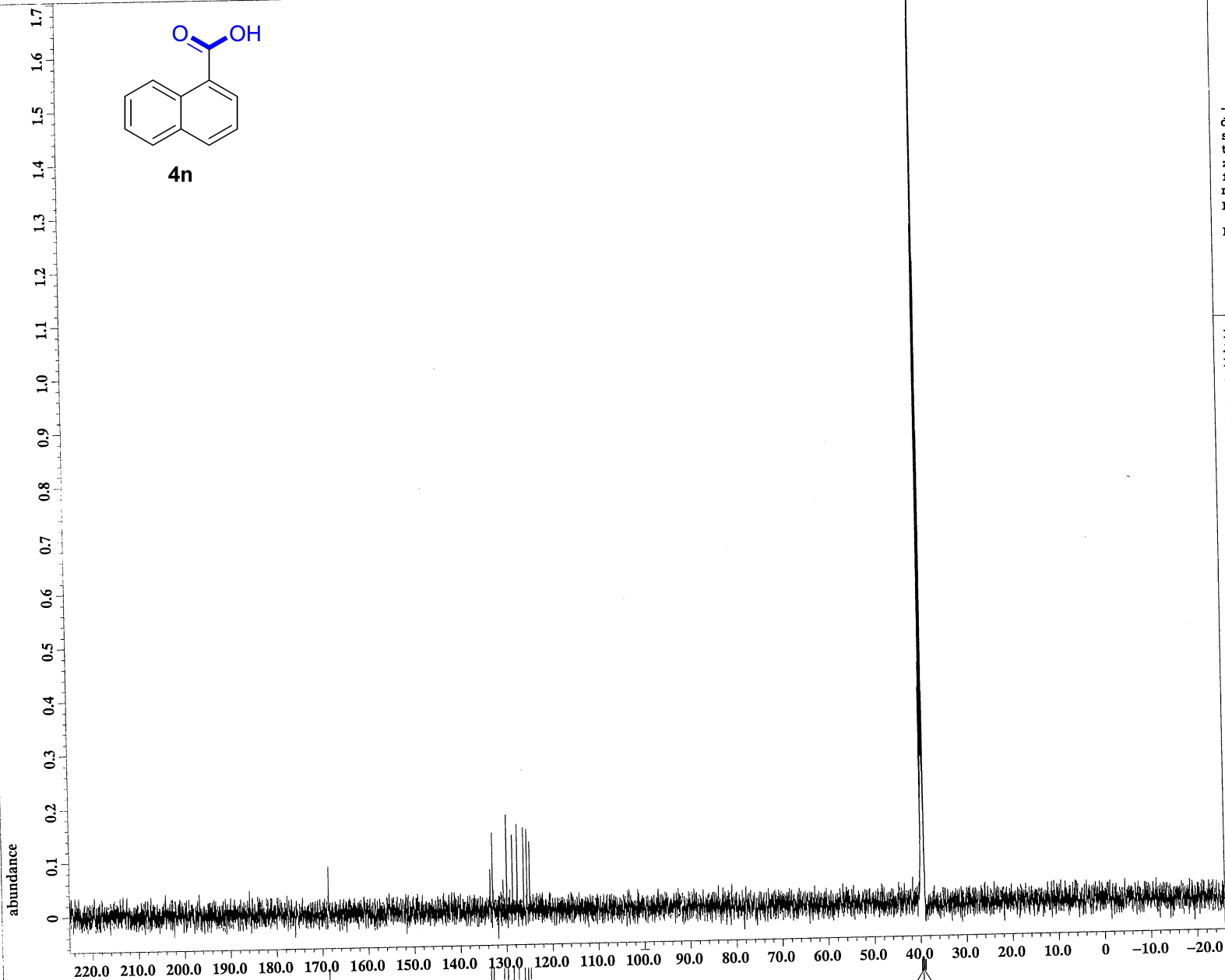
Comment = Exp-R-184-6-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.87293952[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.14555473[Hz]
 X_sweep = 18.76876877[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17[us]
 X_acq_time = 0.87293952[s]
 X_angle = 45[deg]
 X_atn = 3.4[dB]
 X_pulse = 6.585[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 56
 Relaxation_delay = 5[s]
 Repetition_time = 5.87293952[s]
 Temp_get = 21.4[dC]



4n



168.6644

132.9505
129.8770
128.6227
126.2099
125.4918

39.6540
39.5200
39.3764

X : parts per Million : 13C

```

---- 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: Exp-R-184-6-C-1.jdf

```

Filename      = Exp-R-184-6-C-4.jdf
Author        = delta
Experiment    = single_pulse_dec
Sample_id     = Exp-R-184-6-C
Solvent       = DMSO-D6
Creation_time = 18-APR-2019 16:54:59
Revision_time = 18-APR-2019 17:02:58
Current_time  = 18-APR-2019 17:03:16

```

```

Comment       = Exp-R-184-6-C
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units    = [ppm]
Dimensions    = X
Site          = ECA 600
Spectrometer  = DELTA2_NMR

```

```

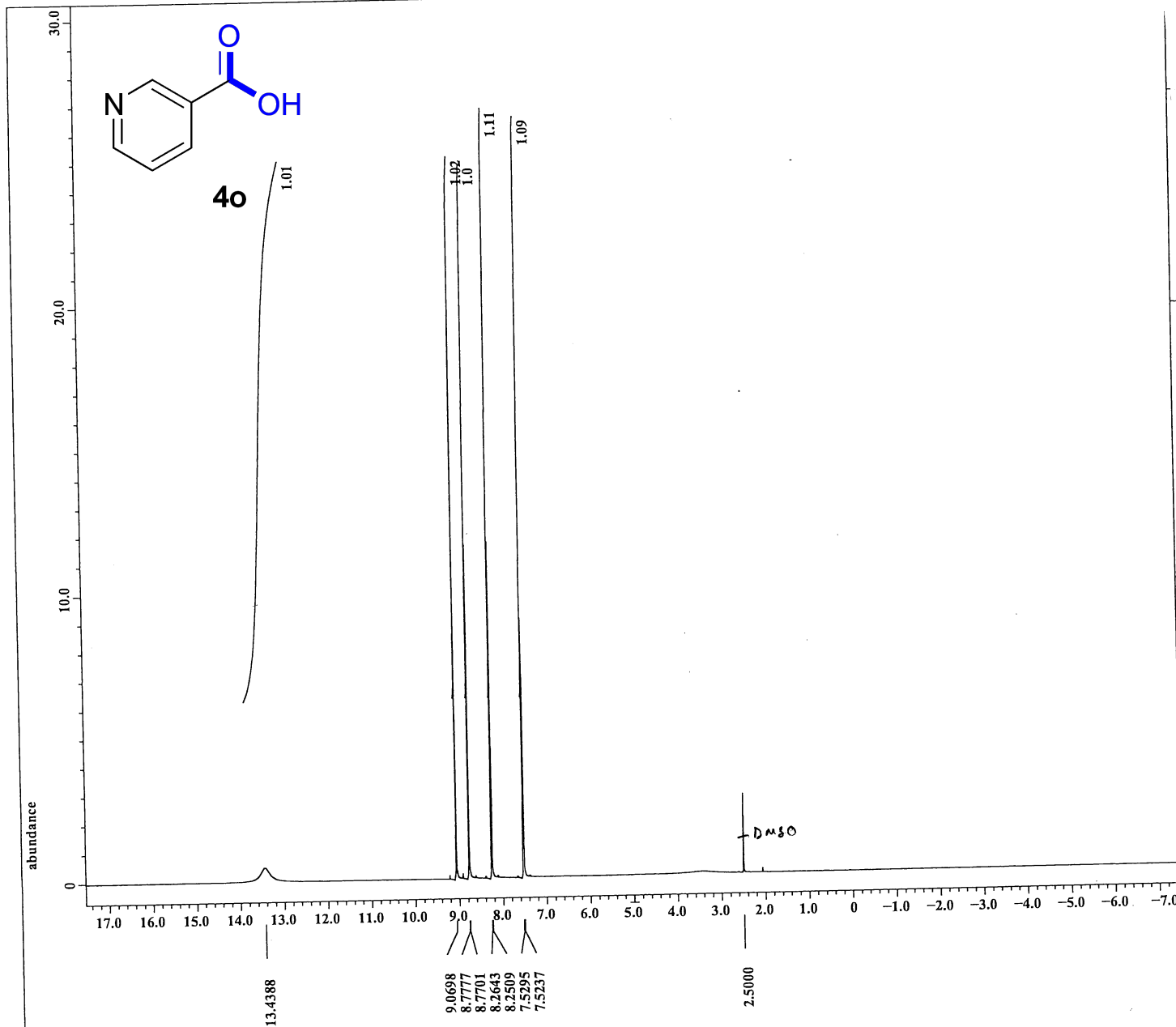
Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485 [kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 43
Total_scans    = 43

```

```

X_90_width    = 12.7[us]
X_acq_time     = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 7.5[dB]
X_pulse        = 4.23333333[us]
Irr_atn_dec    = 18.62[dB]
Irr_atn_noe    = 18.62[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2[s]
Recvr_gain     = 60
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get       = 22[dc]

```



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

Derived from: Exp-R-124-21-1-P-1.jdf

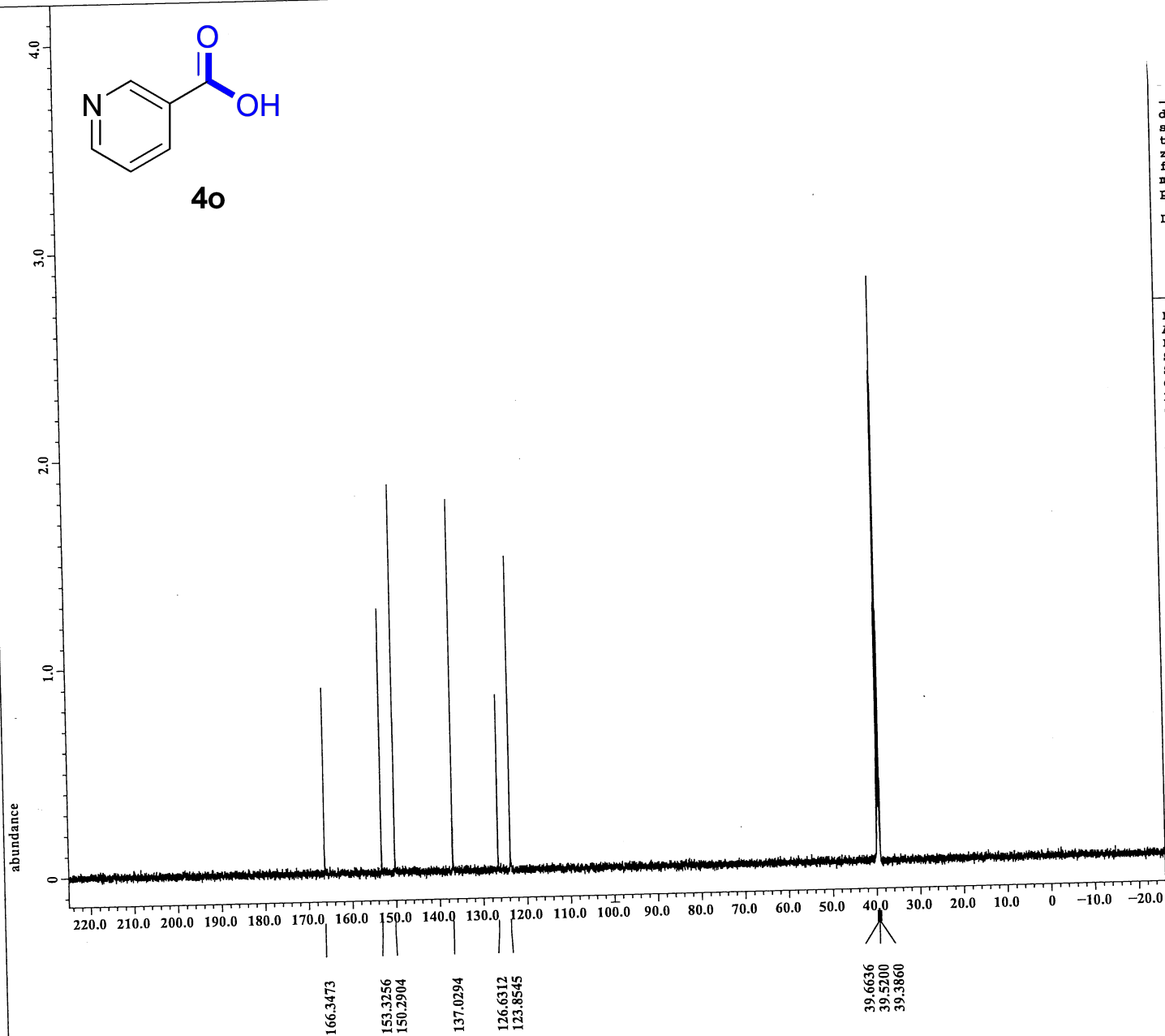
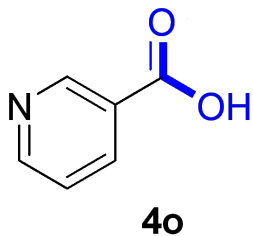
Filename = Exp-R-124-21-1-P-4.jd
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = Exp-R-124-21-1-P
 Solvent = DMSO-D6
 Creation_time = 12-DEC-2018 18:09:11
 Revision_time = 12-DEC-2018 18:14:42
 Current_time = 12-DEC-2018 18:15:03

Comment = Exp-R-124-21-1-P
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M
 X_acq_duration = 0.87293952 [s]
 X_domain = 1H
 X_freq = 600.1723046 [MHz]
 X_offset = 5 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 1.14555473 [Hz]
 X_sweep = 18.76876877 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 13.17 [us]
 X_acq_time = 0.87293952 [s]
 X_angle = 45 [deg]
 X_atn = 3.4 [dB]
 X_pulse = 6.585 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 44
 Relaxation_delay = 5 [s]
 Repetition_time = 5.87293952 [s]
 Temp_get = 21.2 [dc]

X : parts per Million : 1H



X : parts per Million : 13C

---- 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

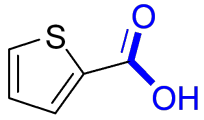
Derived from: Exp-R-124-21-1-C-1.jdf

Filename = Exp-R-124-21-1-C-3.jd
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = Exp-R-124-21-1-C
 Solvent = DMSO-D6
 Creation_time = 12-DEC-2018 18:13:21
 Revision_time = 12-DEC-2018 18:16:36
 Current_time = 12-DEC-2018 18:17:09

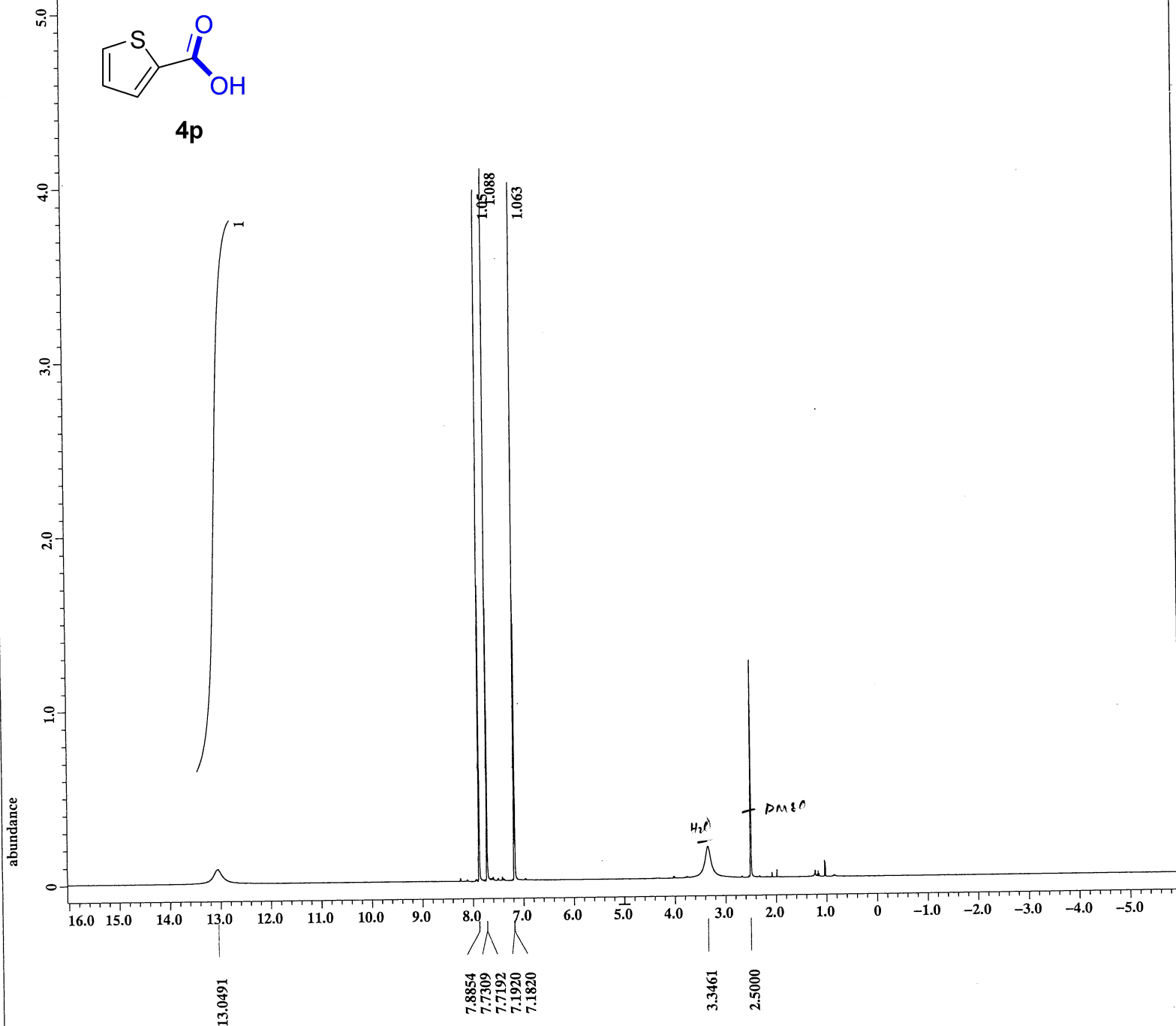
Comment = Exp-R-124-21-1-C
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928 [T] (600 [M])
 X_acq_duration = 0.69206016 [s]
 X_domain = 13C
 X_freq = 150.91343039 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109 [Hz]
 X_sweep = 47.34848485 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 77
 Total_scans = 77

X_90_width = 12.7 [us]
 X_acq_time = 0.69206016 [s]
 X_angle = 30 [deg]
 X_atn = 7.5 [dB]
 X_pulse = 4.23333333 [us]
 Irr_atn_dec = 18.62 [dB]
 Irr_atn_noe = 18.62 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.69206016 [s]
 Temp_get = 21.5 [dC]



4p



```

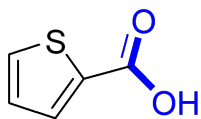
Filename      = R-120-7c-P-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = R-120-7c-P
Solvent      = DMSO-D6
Creation_time = 26-JUL-2018 16:16:18
Revision_time = 26-JUL-2018 17:03:55
Current_time  = 26-JUL-2018 17:04:00

Content      = R-120-7c-P
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 400
Spectrometer = DELTA2_NMR

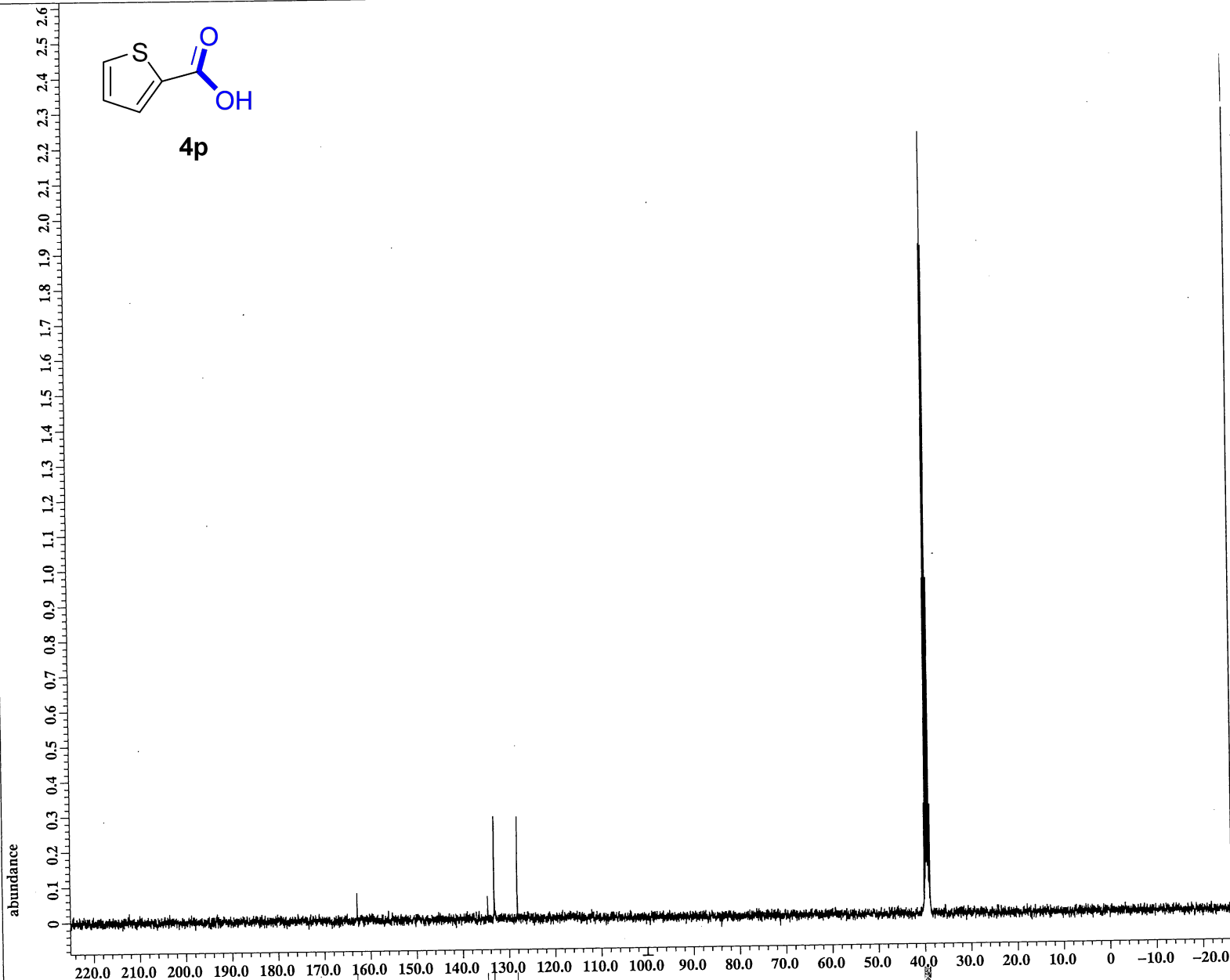
Field_strength = 9.2982153[T] (400[MHz]
X_acq_duration = 1.50470656[s]
X_domain       = 1H
X_freq         = 395.88430144[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.66458141[Hz]
X_sweep        = 10.88850174[kHz]
Irr_domain     = 1H
Irr_freq       = 395.88430144[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 395.88430144[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 10.62[us]
X_acq_time     = 1.50470656[s]
X_angle        = 45[deg]
X_atn          = 9[db]
X_pulse        = 5.31[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_preset  = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 36
Relaxation_delay = 5[s]
Repetition_time = 6.50470656[s]
Temp_get       = 22.8[dC]
  
```

X : parts per Million : 1H



4p



X : parts per Million : ¹³C

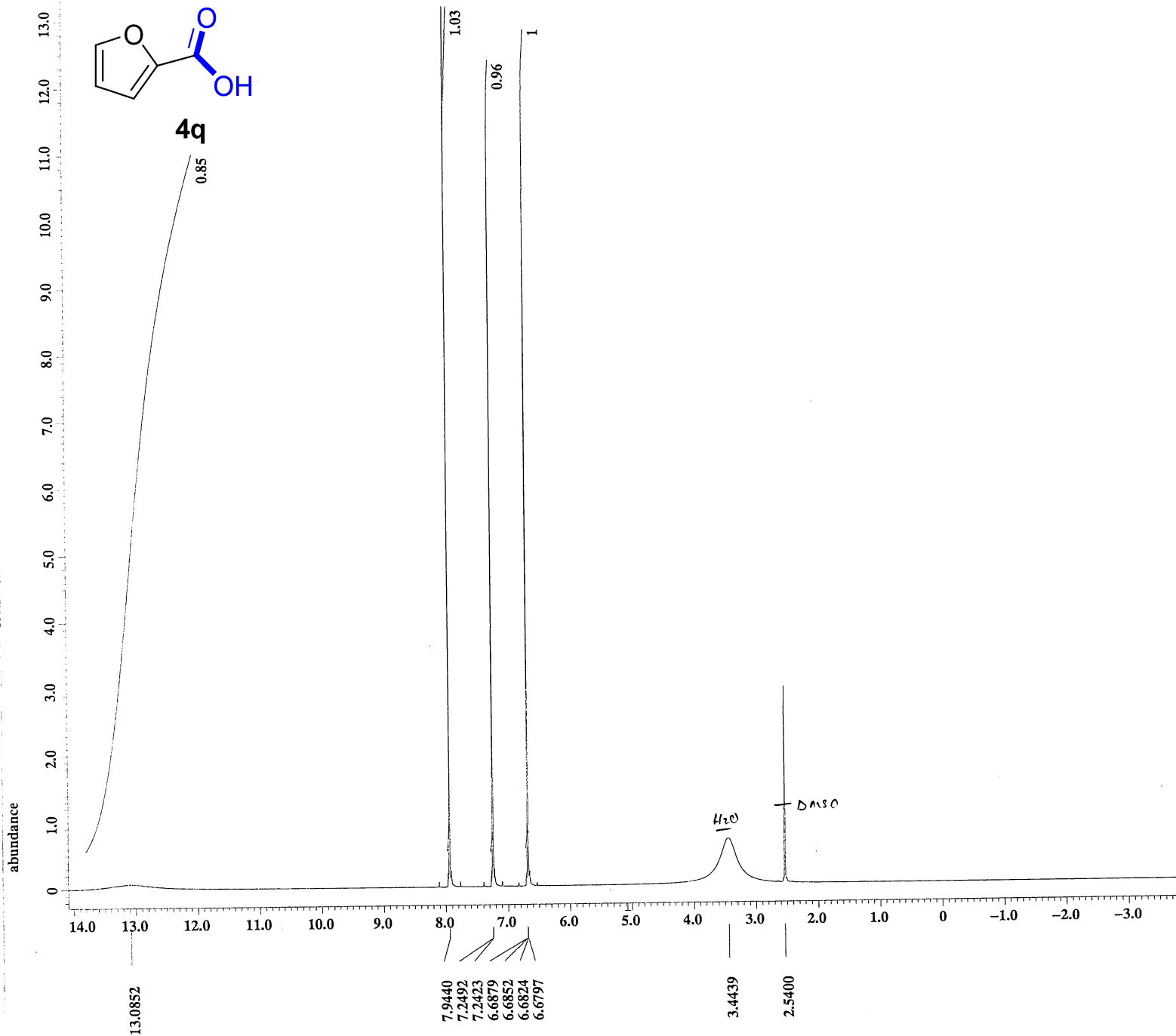
```

Filename      = R-120-7c-C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = R-120-7c-C
Solvent      = DMSO-D6
Creation_time = 26-JUL-2018 16:23:12
Revision_time = 26-JUL-2018 17:05:59
Current_time  = 26-JUL-2018 17:06:14

Content       = R-120-7c-C
Data_format  = 1D_COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.2982153[T] (400[MHz])
X_acq_duration = 1.048576[s]
X_domain       = 13C
X_freq         = 99.54517646[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 0.95367432[Hz]
X_sweep        = 31.25[kHz]
Irr_domain    = 1H
Irr_freq      = 395.88430144[MHz]
Irr_offset    = 5[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 107
Total_scans   = 107

X_90_width    = 9.2[us]
X_acq_time    = 1.048576[s]
X_angle       = 30[deg]
X_atn         = 8.4[dB]
X_pulse       = 3.06666667[us]
Irr_atn_dec   = 29.69[dB]
Irr_atn_noe   = 29.69[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 2[s]
Recvr_gain    = 60
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get      = 23.1[dC]
  
```



X : parts per Million : 1H

```

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

```

Derived from: Exp-AB-R-124-13-H-1.jdf

```

Filename      = Exp-AB-R-124-13-H-5.j
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-AB-R-124-13-H
Solvent      = DMSO-D6
Creation_time = 31-AUG-2020 11:34:37
Revision_time = 31-AUG-2020 11:46:54
Current_time  = 31-AUG-2020 11:46:59

```

```

Comment      = Exp-AB-R-124-13-H
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

```

```

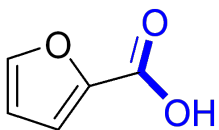
Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 1.21110528[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.82569205[Hz]
X_sweep        = 13.52813853[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

```

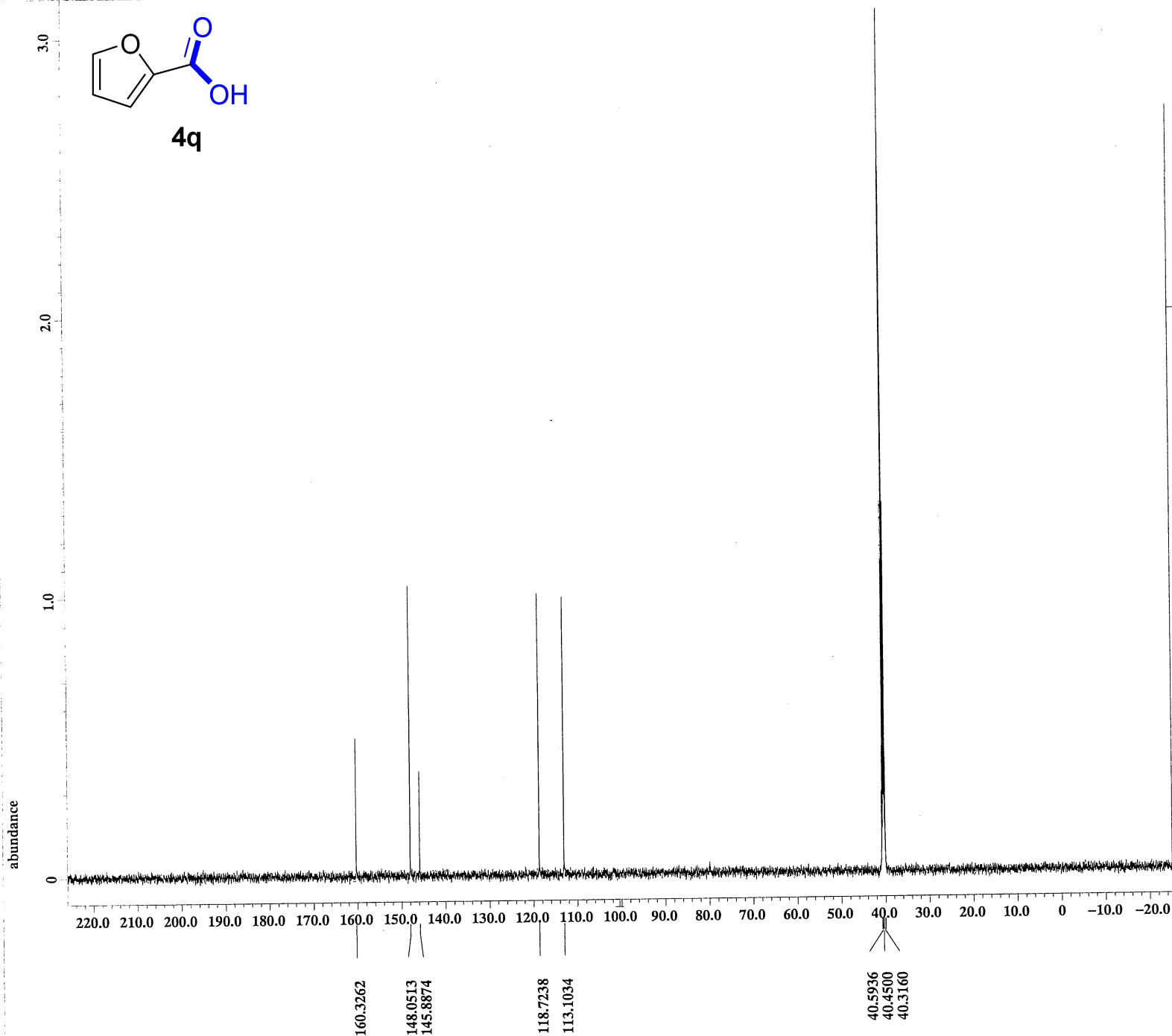
```

X_90_width    = 13.17[us]
X_acq_time     = 1.21110528[s]
X_angle        = 45[deg]
X_atn         = 3.4[dB]
X_pulse        = 6.585[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 48
Relaxation_delay = 5[s]
Repetition_time = 6.21110528[s]
Temp_get       = 21.4[dC]

```

4q



X : parts per Million : 13C

---- 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

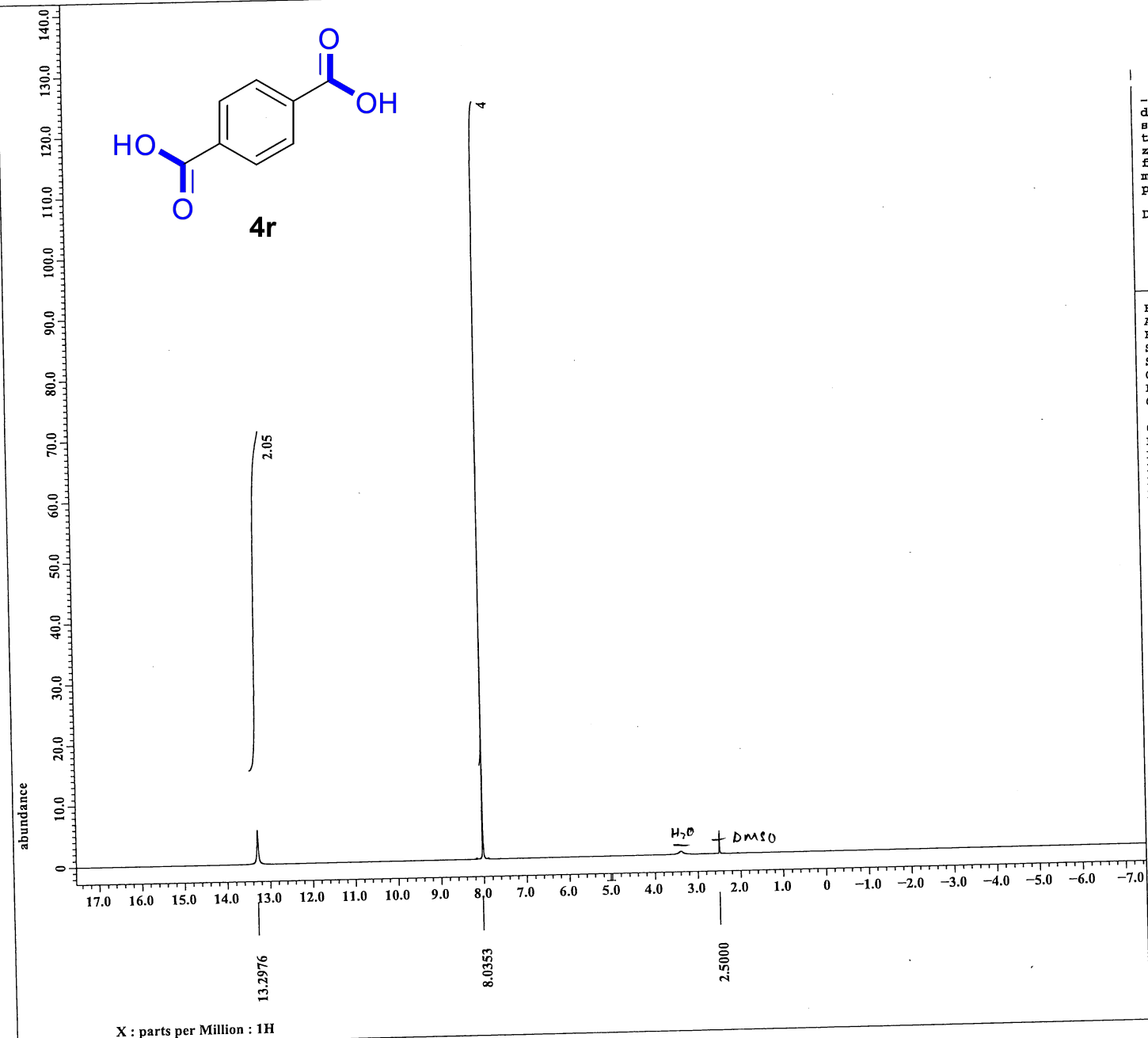
Derived from: Exp-AB-R-124-13-C-1.jdf

Filename = Exp-AB-R-124-13-C-3.j
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = Exp-AB-R-124-13-C
 Solvent = DMSO-D6
 Creation_time = 31-AUG-2020 11:38:39
 Revision_time = 31-AUG-2020 11:44:51
 Current_time = 31-AUG-2020 11:44:55

Comment = Exp-AB-R-124-13-C
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.69206016[s]
 X_domain = 13C
 X_freq = 150.91343039[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109[Hz]
 X_sweep = 47.34848485[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 74
 Total_scans = 74

X_90_width = 12.3[us]
 X_acq_time = 0.69206016[s]
 X_angle = 30[deg]
 X_atn = 7.5[dB]
 X_pulse = 4.1[us]
 Irr_atn_dec = 18.62[dB]
 Irr_atn_noe = 18.62[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 60
 Relaxation_delay = 2[s]
 Repetition_time = 2.69206016[s]
 Temp_get = 22.2[dc]



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

Derived from: Exp-R-182-1-diacid-P-1.jdf

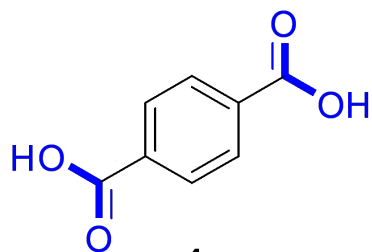
```

Filename      = Exp-R-182-1-diacid-P-
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = Exp-R-182-1-diacid-P
Solvent      = DMSO-D6
Creation_time = 1-APR-2019 17:40:05
Revision_time = 1-APR-2019 17:46:46
Current_time  = 1-APR-2019 17:47:12

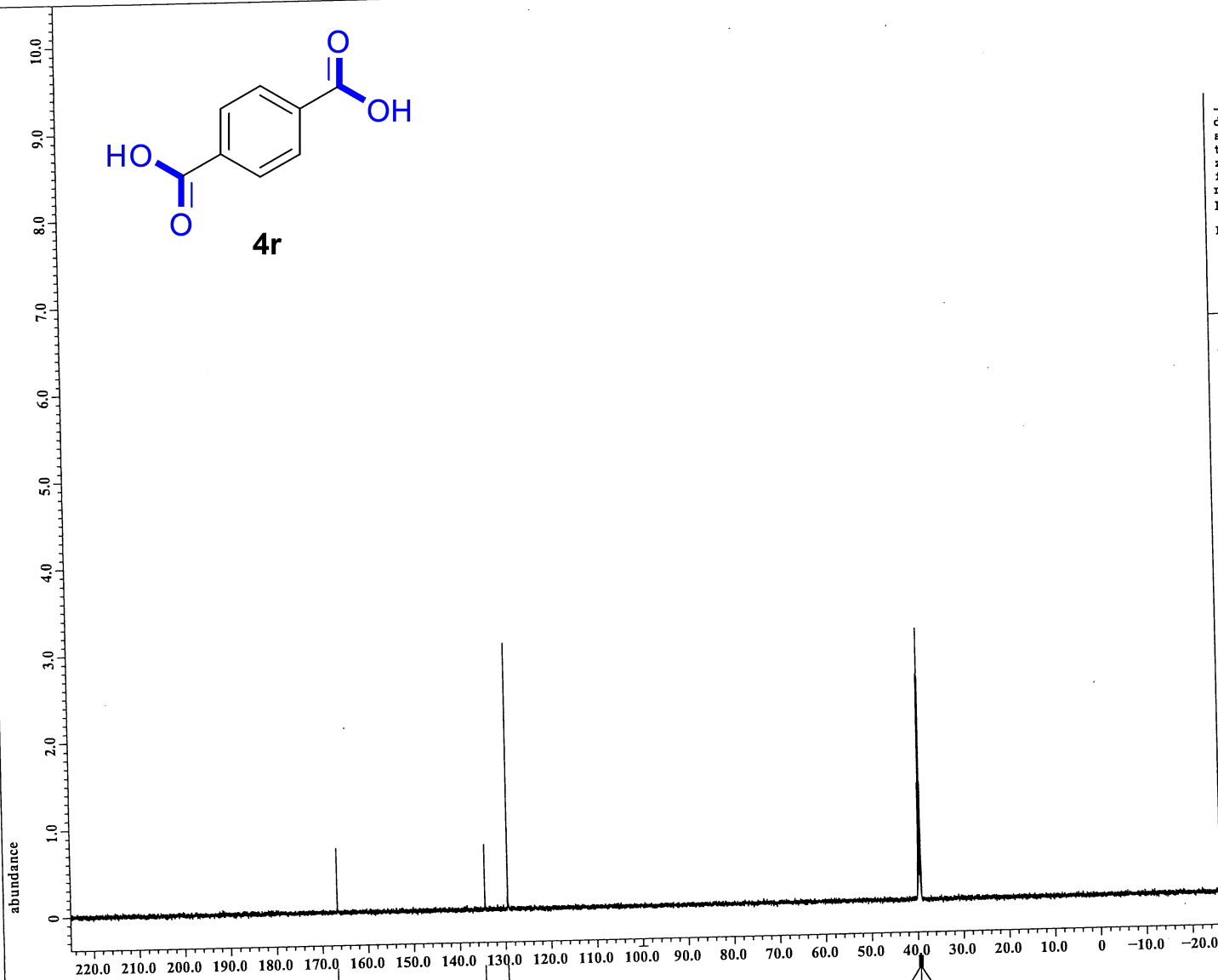
Comment      = Exp-R-182-1-diacid-P
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.87293952[s]
X_domain       = 1H
X_freq         = 600.1723046[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 1.14555473[Hz]
X_sweep        = 18.76876877[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 600.1723046[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 13.17[us]
X_acq_time    = 0.87293952[s]
X_angle       = 45[deg]
X_atn         = 3.4[dB]
X_pulse       = 6.585[us]
Irr_mode      = Off
Tri_mode      = Off
DanTe_preset  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 48
Relaxation_delay = 5[s]
Repetition_time = 5.87293952[s]
Temp_get      = 21.1[dC]
  
```



4r



X : parts per Million : 13C

----- 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: Exp-R-182-1-diacid-C-1.jdf

Filename = Exp-R-182-1-diacid-C-
 Author = delta
 Experiment = single_pulse_dec
 Sample id = Exp-R-182-1-diacid-C
 Solvent = DMSO-D6
 Creation time = 1-APR-2019 17:42:43
 Revision time = 1-APR-2019 17:47:55
 Current time = 1-APR-2019 17:48:20

Comment = Exp-R-182-1-diacid-C
 Data format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field strength = 14.09636928 [T] (600 [M]
 X_acq_duration = 0.69206016 [s]
 X_domain = 13C
 X_freq = 150.91343039 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109 [Hz]
 X_sweep = 47.34848485 [kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 43
 Total_scans = 43

X_90_width = 12.7 [us]
 X_acq_time = 0.69206016 [s]
 X_angle = 30 [deg]
 X_atn = 7.5 [dB]
 X_pulse = 4.23333333 [us]
 Irr_atn_dec = 18.62 [dB]
 Irr_atn_noe = 18.62 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.69206016 [s]
 Temp_get = 21.6 [dC]