# Supporting Information

Synthesis of Alkyl Aryl Ketones by Pd/Light Induced Carbonylative Cross-Coupling of Alkyl Iodides and Arylboronic Acids

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**General Information**

Thin layer chromatography (TLC) was performed on Merck precoated plates (silica gel 60 F254, Art 5715, 0.25 mm) and were visualized by fluorescence quenching under UV light or by staining with *p*-anisaldeyde/AcOH/$H_2SO_4$/EtOH, or $12MoO_3.H_3PO_4$/EtOH. The products were purified by flash chromatography on silica gel (Kanto Chem. Co. Silica Gel 60N (spherical, neutral, 40-50 μm)) and, if necessary, were further purified by recycling preparative HPLC (Japan Analytical Industry Co. Ltd., LC-918) equipped with GPC columns (JAIGEL-1H + JAIGEL-2H columns) using $CHCl_3$ as eluent. $^1$H NMR spectra were recorded with a JEOL JNM-ECS400 (400 MHz) spectrometer and referenced to the peak of the residual TMS at 0.00 ppm. $^{13}$C NMR spectra were recorded with a JEOL JNM-ECS400 (100 MHz) spectrometer and referenced to the solvent peak at 77.16 ppm. Splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Infrared spectra were recorded on a JASCO FT/IR-4100 spectrometer and are reported as wavenumber ($cm^{-1}$). Conventional and high-resolution mass spectra were recorded with a JEOL MS700 spectrometer.

**Typical procedure for the synthesis of nonanophenone** (**3a**)

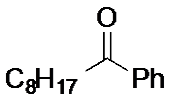
A magnetic stirring bar, iodooctane (**1a**) (121.9mg, 0.5 mmol), phenylboronic acid (**2a**) (91.7mg, 0.75 mmol), $PdCl_2(PPh_3)_2$ (16.4 mg, 0.025 mmol), $K_2CO_3$ (139.1 mg, 1.0 mmol), $C_6H_6$ (4 mL), and $H_2O$ (2 mL) were placed in a stainless steel autoclave for photoreaction equipped with an inserted Pyrex glass liner. The autoclave was closed, purged three times with carbon monoxide, pressurized with 45 atm of CO and then irradiated by Xenon arc lamp (500 W) with stirring for 16 h. Excess CO was discharged at room temperature after the reaction. The reaction mixture was poured into water (20 mL) and extracted with ether (20 mL × 3). The combined ether layer was washed with brine and dried over $MgSO_4$, then filtered and concentrated *in vacuo* to give a residue, which was subjected to silica gel column chromatography using hexan/EtOAc = 250/1 as eluent affording nonanophenone (**3a**) (100.6 mg, 91%)

**Procedure for the synthesis of ethyl 4-benzoyldecanoate** (**6**)

A magnetic stirring bar, ethyl iodoacetate (**4**) (110.0 mg, 0.5 mmol), 1-octene (**5**) (566.9 mg, 5.1 mmol), phenylboronic acid (**2a**) (94.1 mg, 0.77 mmol), $PdCl_2(PPh_3)_2$ (16.1 mg, 0.025 mmol), $K_2CO_3$ (136.2 mg, 1.0 mmol), $C_6H_6$ (4 mL) and $H_2O$ (2 mL) were placed in a stainless steel autoclave for photoreaction equipped with an inserted Pyrex glass liner. The autoclave was closed, purged three times with carbon monoxide, pressurized with 45 atm of CO and then irradiated by Xenon arc lamp (500 W) with stirring for 16 h. Excess CO was discharged at room temperature after the reaction. The reaction mixture was poured into water (20 mL) and extracted with ether (20 mL × 3). The

combined ether layer was washed with brine, and dried over $MgSO_4$, then filtered and concentrated *in vacuo* to give a residue, which was subjected to silica gel column chromatography using hexan/EtOAc = 200/1 as eluent affording ethyl 4-benzoyldecanoate (**6**) (96.5 mg, 62 %)

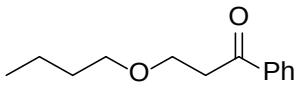
**Nonanophenone** (**3a**)



This compound is previously known and commercially available: Vautravers, N. R.; Regent, D. D.; Breit, B. *Chem. Commun.* **2011**, 47, 6635.

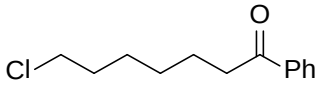
Colorless oil; $^1$H-NMR ($CDCl_3$, 400 MHz) δ 7.97-7.95 (m, 2H), 7.57-7.53 (m, 1H), 7.48-7.44 (m, 2H), 2.98-2.95 (m, 2H), 1.79-1.70 (m, 2H), 1.41-1.27 (m, 10H), 0.88 (m, 3H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 200.61, 137.14, 132.91, 128.60, 128.11, 38.70, 31.93, 29.54, 29.46, 29.26, 24.44, 22.74, 14.19.

**3-Butoxy-1-phenylpropan-1-one** (**3b**)



Colorless oil; $^1$H-NMR ($CDCl_3$, 400 MHz) δ 7.98-7.96 (m, 2H), 7.59-7.55 (m, 1H), 7.49-7.45 (m, 2H), 3.87-3.84 (m, 2H), 3.47 (t, *J* = 6.8 Hz, 2H), 3.28-3.24 (m, 2H), 1.57-1.51 (m, 2H), 1.38-1.31 (m, 2H), 0.92-0.88 (m, 3H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 198.65, 137.13, 133.21, 128.68, 128.24, 71.21, 66.11, 39.04, 31.83, 19.40, 14.02; IR (neat) 2958 $cm^{-1}$, 1682 $cm^{-1}$, 1112 $cm^{-1}$; MS (relative intensity) m/z 206 ($M^+$, 13), 151 (34), 133 (66), 105 (100), 77 (78); HRMS (EI) m/z calcd for $C_{13}H_{18}O_2$ 206.1307, found 206.1308.

**7-Chloro-1-phenylheptan-1-one** (**3c**)

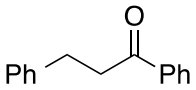


This compound is previously known and commercially available: Rieke, R. D.; Stack, D. E.; Dawson, B. T.; Wu, T.-C. *J. Org. Chem.* **1993**, *58*, 2483.

White solid (m.p. = 32.7-33.6 °C); $^1$H-NMR ($CDCl_3$, 400 MHz) δ 7.97-7.95 (m, 2H), 7.58-7.54 (m, 1H), 7.48-7.45 (m, 2H), 3.54 (t, *J* = 6.6 Hz, 2H), 3.00-2.97 (m, 2H), 1.82-1.73 (m, 4H), 1.50-1.41 (m, 4H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 200.40, 137.11, 133.08, 128.69, 128.14, 45.18, 38.49, 32.52,

28.67, 26.84, 24.17.

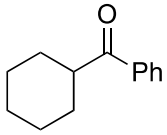
**1,3-Diphenyl-propan-1-one** (**3d**)




This compound is previously known: Colbon, P.; Ruan, J.; Purdie, M.; Xiao, J. *Org. Lett*. **2010**, *12*, 3670.

White solid (m.p. = 66.9-68.1 °C); $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.97-7.95 (m, 2H), 7.56-7.47 (m, 1H), 7.45-7.43 (m, 2H), 7.30-7.21 (m, 5H), 3.33-3.29 (m, 2H), 3.09-3.05 (m, 2H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 199.30, 141.38, 136.91, 133.17, 128.70, 128.63, 128.53, 128.13, 126.23, 40.55, 30.20.

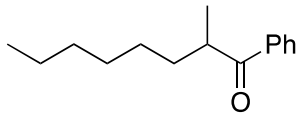
**Cyclohexylphenylmethanone** (**3e**)




This compound is previously known and commercially available: Hsieh, J.-C.; Chem, Y.-C.; Cheng, A.-Y.; Tseng, H.-C. *Org. Lett.* **2012**, *14*, 1282.

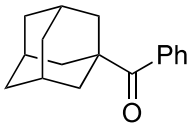
White solid (m.p. = 55.6-56.1 °C); $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.96-7.94 (m, 2H), 7.56-7.53 (m, 1H), 7.48-7.44 (m, 2H), 3.30-3.23 (m, 1H), 1.91-1.83 (m, 3H), 1.78-1.72 (m, 2H), 1.57-1.21 (m, 5H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 203.94, 136.38, 132.80, 128.65, 128.32, 45.67, 29.49, 26.05, 25.93.

**2-Methyl-1-phenyloctan-1-one** (**3f**)




Colorless oil; $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.97-7.94 (m, 2H), 7.58-7.54 (m, 1H), 7.49-7.45 (m, 2H), 3.51-3.42 (m, 1H), 1.83-1.76 (m, 1H), 1.48-1.41 (m, 1H), 1.34-1.22 (m, 8H), 1.19 (d, $J$ = 6.8 Hz, 3H), 0.86 (t, $J$ = 6.8 Hz, 3H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 204.68, 136.87, 132.89, 128.70, 128.33, 40.67, 33.85, 31.80, 29.51, 27.49, 22.70, 17.34, 14.17; IR (neat) 2930 $cm^{-1}$, 2856 $cm^{-1}$, 1682 $cm^{-1}$, 703 $cm^{-1}$; MS (relative intensity) m/z 218 ($M^+$, 10), 134 (48), 105 (100), 77 (40); HRMS (EI) m/z calcd for $C_{15}H_{22}O$ 218.1671, found 218.1676.

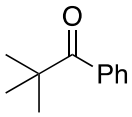
**1-Benzoyladamantane** (**3g**)




This compound is previously known: Lo Fiego, M. J.; Lockhart, M. T.; Chopa, A. B. *J. Organomet. Chem.* **2009**, *694*, 3674.

White solid (m.p. = 49.3-50.1 °C); $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.55-7.53 (m, 2H), 7.45-7.36 (m, 3H), 2.10-2.00 (m, 10H), 1.80-1.69 (m, 5H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 210.22, 139.65, 130.21, 128.00, 127.17, 46.95, 39.14, 36.59, 28.18.

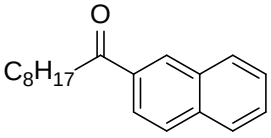
**2,2-Dimethyl-1-phenyl-propan-1-one** (**3h**)




This compound is previously known: Zhu, Y.; Zhao, B.; Shi, Y. *Org. Lett.* **2013**, *15*, 992.

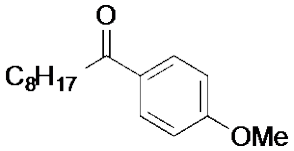
Colorless oil; $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.70-7.68 (m, 2H), 7.48-7.38 (m, 3H), 1.35 (s, 9H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 209.48, 138.72, 130.95, 128.18, 127.96, 28.15.

**1-(2-Naphthyl)-nonan-1-one** (**3i**)




White solid (m.p. = 54.1-54.7 °C); $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 8.47 (s, 1H), 8.05-8.03 (m, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.91-7.87 (m, 2H), 7.61-7.51 (m, 2H), 3.12-3.08 (m, 2H), 1.85-1.76 (m, 2H), 1.44-1.22 (m, 10H), 0.90-0.87 (m, 3H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 200.76, 135.64, 134.55, 132.69, 129.75, 129.67, 128.52, 128.47, 127.90, 126.84, 124.11, 38.87, 31.99, 29.63, 29.58, 29.35, 24.69, 22.82, 14.27; IR (neat) 2933 $cm^{-1}$, 2849 $cm^{-1}$, 1683 $cm^{-1}$, 1463 $cm^{-1}$, 803 $cm^{-1}$, 755 $cm^{-1}$; MS (relative intensity) m/z 268 ($M^+$, 19), 170 (100), 155 (83), 127 (49); HRMS (EI) m/z calcd for $C_{19}H_{24}O$ 268.1827, found 268.1833.

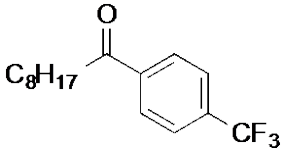
**1-(4-Methoxyphenyl)nonan-1-one** (**3j**)




This compound is previously known: Vautravers, N. R.; Reqert, D. D.; Breit, B. *Chem. Commun.* **2011**, *47*, 6635.

White solid (m.p. = 43-44 °C); $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.94 (d, *J* = 8.0 Hz, 2H), 6.93 (d, *J* = 7.6 Hz, 2H), 3.87 (s, 3H), 2.93-2.88 (m, 2H), 1.79-1.69 (m, 2H), 1.42-1.20 (m, 10H), 0.88 (t, J = 6.8 Hz, 3H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 199.29, 163.36, 130.38, 130.24, 113.72, 55.50, 38.38, 31.94, 29.56, 29.53, 29.27, 24.71, 22.74, 14.19.

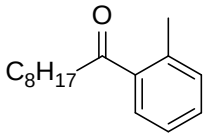
**1-(4-Trifluoromethylphenyl)nonan-1-one** (**3k**)




This Compound is previously known: Dohi, S.: Moriyama, K.; Togo, H. *Tetrahedron* **2012**, *68*, 6557.

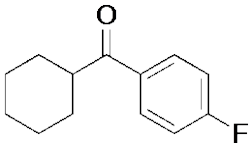
White solid (m.p. = 35.5-36.1 °C); $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 8.07-8.05 (m, 2H), 7.74-7.72 (m, 2H), 3.00-2.97 (m, 2H), 1.80-1.71 (m, 2H), 1.39-1.27 (m, 10H), 0.88 (t, *J* = 6.8 Hz, 3H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 199.70, 139.34 (q, $J_{C\text{-}F}$ = 32.5 Hz), 128.51, 125.79 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.77 (q, $J_{C\text{-}F}$ = 270.2 Hz), 39.08, 31.97, 29.56, 29.44, 29.30, 24.28, 22.80, 14.24; $^{19}$F-NMR ($CDCl_3$, 377 MHz) δ -62.98.

**1-(*o*-Tolyl)nonan-1-one** (**3l**)



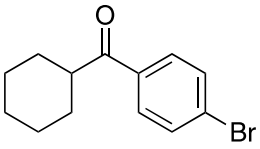

Colorless oil; $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.62-7.60 (m, 1H), 7.37-7.34 (m, 1H), 7.26-7.23 (m, 2H), 2.90-2.86 (m, 2H), 2.48 (s, 3H), 1.75-1.66 (m, 2H), 1.39-1.27 (m, 10H), 0.89-0.87 (m, 3H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 205.09, 138.46, 137.88, 131.96, 131.09, 128.36, 125.71, 41.80, 31.95, 29.56, 29.45, 29.29, 24.55, 22.77, 21.30, 14.22; IR (neat) 2925 cm$^{-1}$, 2854 cm$^{-1}$, 1687 cm$^{-1}$, 1456 cm$^{-1}$, 753 cm$^{-1}$; MS (relative intensity) m/z 232 ($M^+$, 8), 134 (47), 119 (100), 91 (59); HRMS (EI) m/z calcd for $C_{16}H_{24}O$ 232.1827, found 232.1820.

**Cyclohexyl-(4-fluorophenyl)methanone** (**3m**)



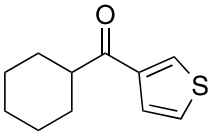
Colorless oil; $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.99-7.95 (m, 2H), 7.13 (t, $J$ = 8.4 Hz, 2H), 3.25-2.17 (m, 1H), 1.90-1.82 (m, 4H), 1.78-1.70 (m, 1H), 1.55-1.22 (m, 5H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 202.36, 165.65 (d, $J_{C-F}$ = 251.1 Hz), 132.76 (d, $J_{C-F}$ = 2.9 Hz), 130.97 (d, $J_{C-F}$ = 8.6 Hz), 115.74 (d, $J_{C-F}$ = 22.0 Hz), 45.68, 29.52, 26.03, 25.94; $^{19}$F-NMR ($CDCl_3$, 377 MHz) δ -105.87; IR (neat) 2943 cm$^{-1}$, 2855 cm$^{-1}$, 1681 cm$^{-1}$, 1236 cm$^{-1}$, 843 cm$^{-1}$; MS (relative intensity) m/z 206 ($M^+$, 25), 151 (20), 123 (100), 95 (21); HRMS (EI) m/z calcd for $C_{13}H_{15}FO$ 206.1107, found 206.1102.

**Cyclohexyl-(4-bromophenyl)methanone** (**3n**)



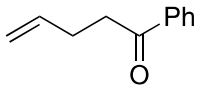
White solid (m.p. = 76.5-77.0 °C); $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.81 (d, $J$ = 8.4 Hz, 2H), 7.60 (d, $J$ = 8.0 Hz, 2H), 3.30-3.23 (m, 1H), 1.90-1.81 (m, 4H), 1.79-1.70 (m, 1H), 1.54-1.21 (m, 5H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 202.92, 135.11, 132.00, 129.95, 127.94, 45.71, 29.45, 26.01, 25.91; IR (KBr) 2928 cm$^{-1}$, 1680 cm$^{-1}$, 833 cm$^{-1}$; MS (relative intensity) m/z 268 ($M^+$, 20), 266 ($M^+$, 21), 187 (40), 185 (100), 183 (99), 157 (20), 155 (20); HRMS (EI) m/z calcd for $C_{13}H_{15}{}^{79}BrO$ 266.0306, found 266.0297.

**Cyclohexyl-(3-thienyl)methanone** (**3o**)



White solid (m.p. = 55.0-55.8 °C); $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 8.05 (t, $J$ = 1.4 Hz, 1H), 7.55 (d, $J$ = 4.8 Hz, 1H), 7.32-7.30 (m, 1H), 3.10-3.03 (m, 1H), 1.90-1.81 (m, 4H), 1.76-1.70 (m, 1H), 1.56-1.21 (m, 5H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 198.31, 141.64, 131.79, 127.38, 126.32, 47.71, 29.45, 25.98, 25.90; IR (KBr) 1654 cm$^{-1}$, 2850 cm$^{-1}$; MS (relative intensity) m/z 194 ($M^+$, 45), 111 (100); HRMS (EI) m/z calcd for $C_{11}H_{14}OS$ 194.0765, found 194.0758.

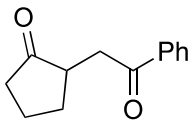
**1-Phenyl-4-penten-1-one** (**3p**)




This product is previously known and commercially available: Pirtsch, M.; Paria, S.; Matsuno, T.; Reiser, O.; Isobe, H. *Chem. -Eur. J.* **2012**, *18*, 7336.

Colorless oil; $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.98-7.96 (m, 2H), 7.60-7.54 (m, 1H), 7.49-7.45 (m, 2H), 5.92 (ddt, *J* = 16.8 Hz, 10.0 Hz, 6.4 Hz, 1H), 5.09 (ddd, *J* = 16.8 Hz, 3.2 Hz, 1.6 Hz, 1H), 5.02 (ddd, *J* = 10.0 Hz, 3.2 Hz, 1.6 Hz, 1H), 3.10-3.07 (m, 2H), 2.52-2.47 (m, 2H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 199.54, 137.41, 137.01, 133.12, 128.70, 128.13, 115.40, 37.84, 28.24.

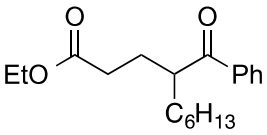
**2-Phenacyl-cyclopentanone** (**3q**)



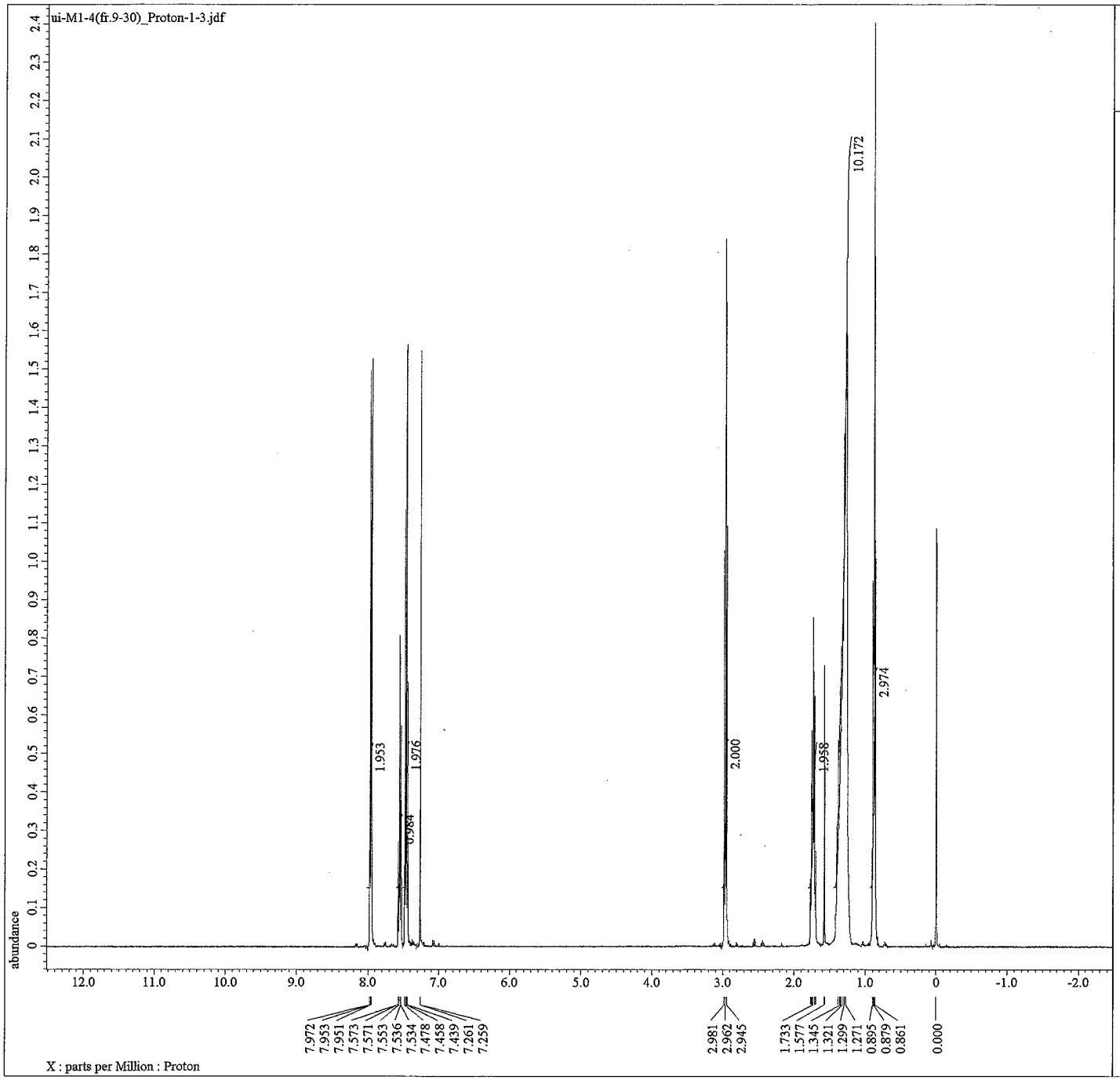

This product is previously known; Thompson, B. B.; Montgomery, J. *Org. Lett*. **2011**, *13*, 3289.

Colorless oil; $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.96 (d, *J* = 7.6 Hz, 2H), 7.59-7.56 (m, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 3.54 (dd, *J* = 3.2 Hz, 18.4 Hz, 1H), 3.06 (dd, *J* = 8.4 Hz, 17.6 Hz, 1H), 2.61-2.69 (m, 1H), 2.45-2.26 (m, 3H), 2.13-2.06 (m, 1H), 1.95-1.81 (m, 1H), 1.69-1.57 (m, 1H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 220.53, 198.04, 136.63, 133.32, 128.69, 128.10, 45.15, 38.70, 37.64, 29.76, 20.91.

**Ethyl 4-benzoyldecanoate** (**6**)




Colorless oil; $^{1}$H-NMR ($CDCl_3$, 400 MHz) δ 7.97-7.95 (m, 2H), 7.59-7.55 (m, 1H), 7.49-7.45 (m, 2H), 4.09 (q, *J* = 6.9 Hz, 2H), 3.55-3.49 (m, 1H), 2.38-2.30 (m, 1H), 2.26-2.20 (m, 1H), 2.18-2.06 (m, 1H), 1.90-1.81 (m, 1H), 1.77-1.72 (m, 1H), 1.51-1.45 (m, 1H), 1.26-1.19 (m, 11H), 0.86-0.82 (m, 3H); $^{13}$C-NMR ($CDCl_3$, 100 MHz) δ 203.90, 173.40, 137.91, 133.13, 128.77, 128.32, 60.43, 45.02, 32.56, 31.97, 31.69, 29.48, 27.37, 26.93, 22.64, 14.27, 14.13; IR (neat) 1216 $cm^{-1}$, 1680 $cm^{-1}$, 1731 $cm^{-1}$, 2929 $cm^{-1}$, 704 $cm^{-1}$; MS (relative intensity) m/z 304 ($M^{+}$, 3), 259 (10), 220 (29), 105 (100), 77 (19); HRMS (EI) m/z calcd for $C_{19}H_{28}O_3$ 304.2038, found 304.2031.




JEOL RESONANCE

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| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-M1-4(fr.9-30) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 10-APR-2013 22:56:01 |
| Revision_Time | = 10-APR-2013 22:54:48 |
| Current_Time | = 10-APR-2013 22:56:31 |
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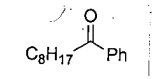
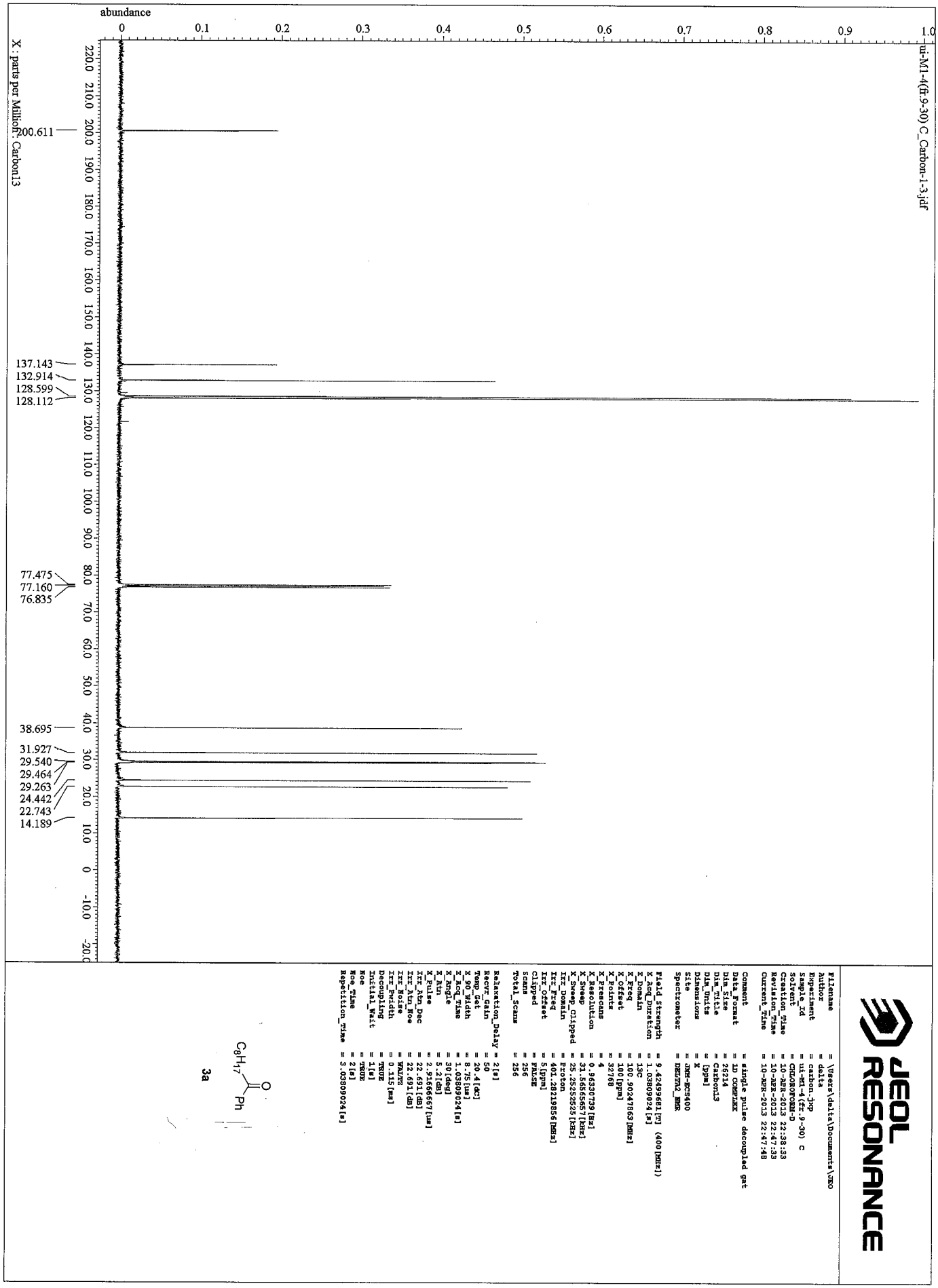
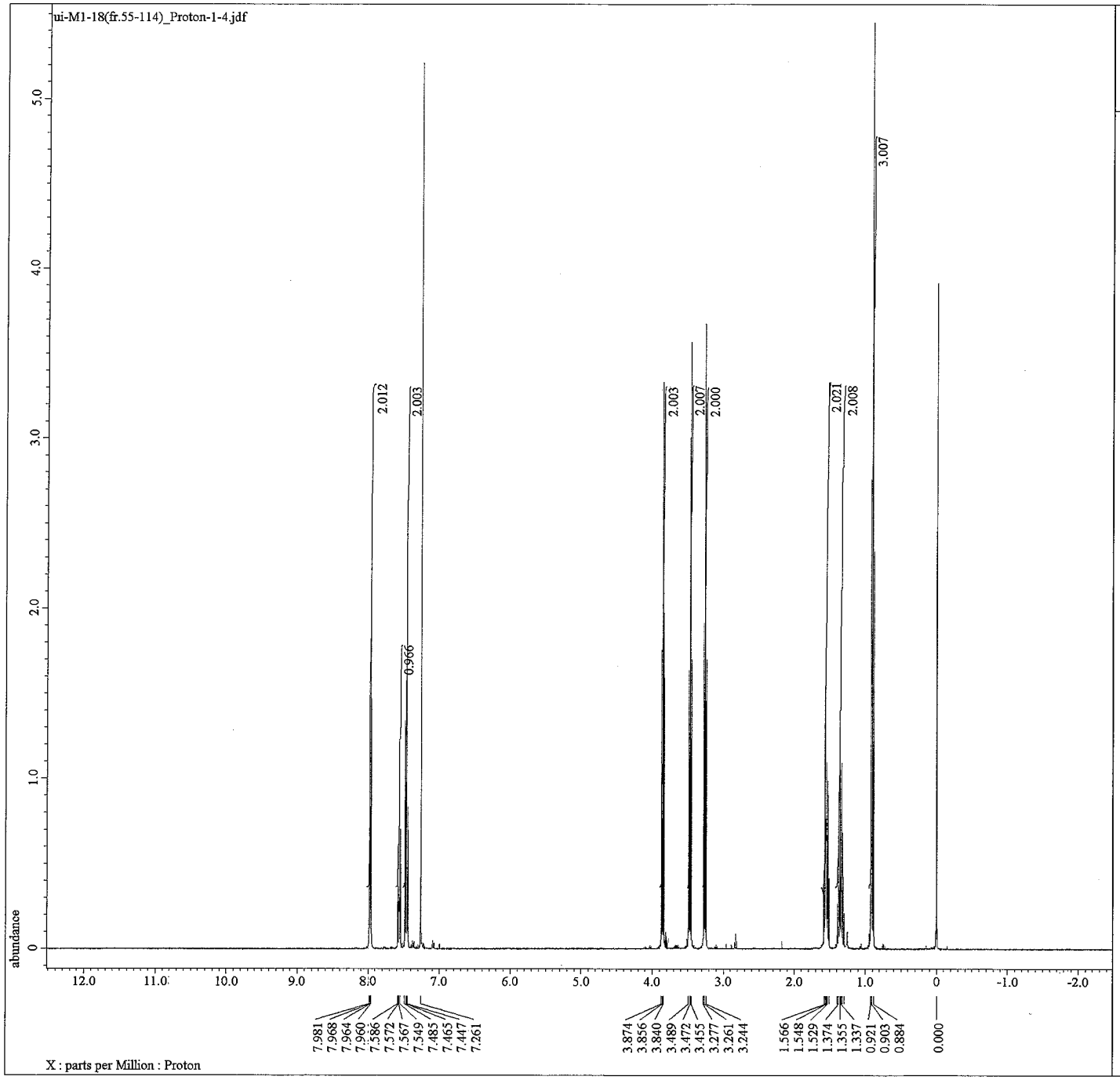
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.1757952[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 42 |
| Temp_Get | = 20.6[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.1757952[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.1757952[s] |




**3a**


abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
ui-M1-4(ff.9-30) C_Carbon-1-3.jdf
X : parts per Million: Carbon13
200.611
137.143
132.914
128.599
128.112
77.475
77.160
76.835
38.695
31.927
29.540
29.464
29.263
24.442
22.743
14.189
JEOL RESONANCE
Filename = \Users\delta\Documents\NMR
Author = delta
Experiment = carbon.jxp
Sample_Id = ui-M1-4(ff.9-30) C
Solvent = CHLOROFORM-D
Creation_Time = 10-APR-2013 22:38:33
Revision_Time = 10-APR-2013 22:47:33
Current_Time = 10-APR-2013 22:47:48
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681[T] (400[MHz])
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.90247863[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[Hz]
X_Sweep_Clipped = 25.25252525[Hz]
X_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.4[dC]
X_90_Width = 8.75[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 5.2[dB]
X_Pulse = 2.91666667[us]
Irr_Atn_Dec = 22.69[dB]
Irr_Atn_Noe = 22.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = CWUP
Initial_Wait = 1[s]
Noe = CWUP
Noe_Time = 2[s]
Repetition_Time = 3.03809024[s]
C8H17
O
Ph
3a




JEOL RESONANCE

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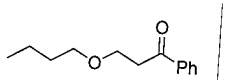
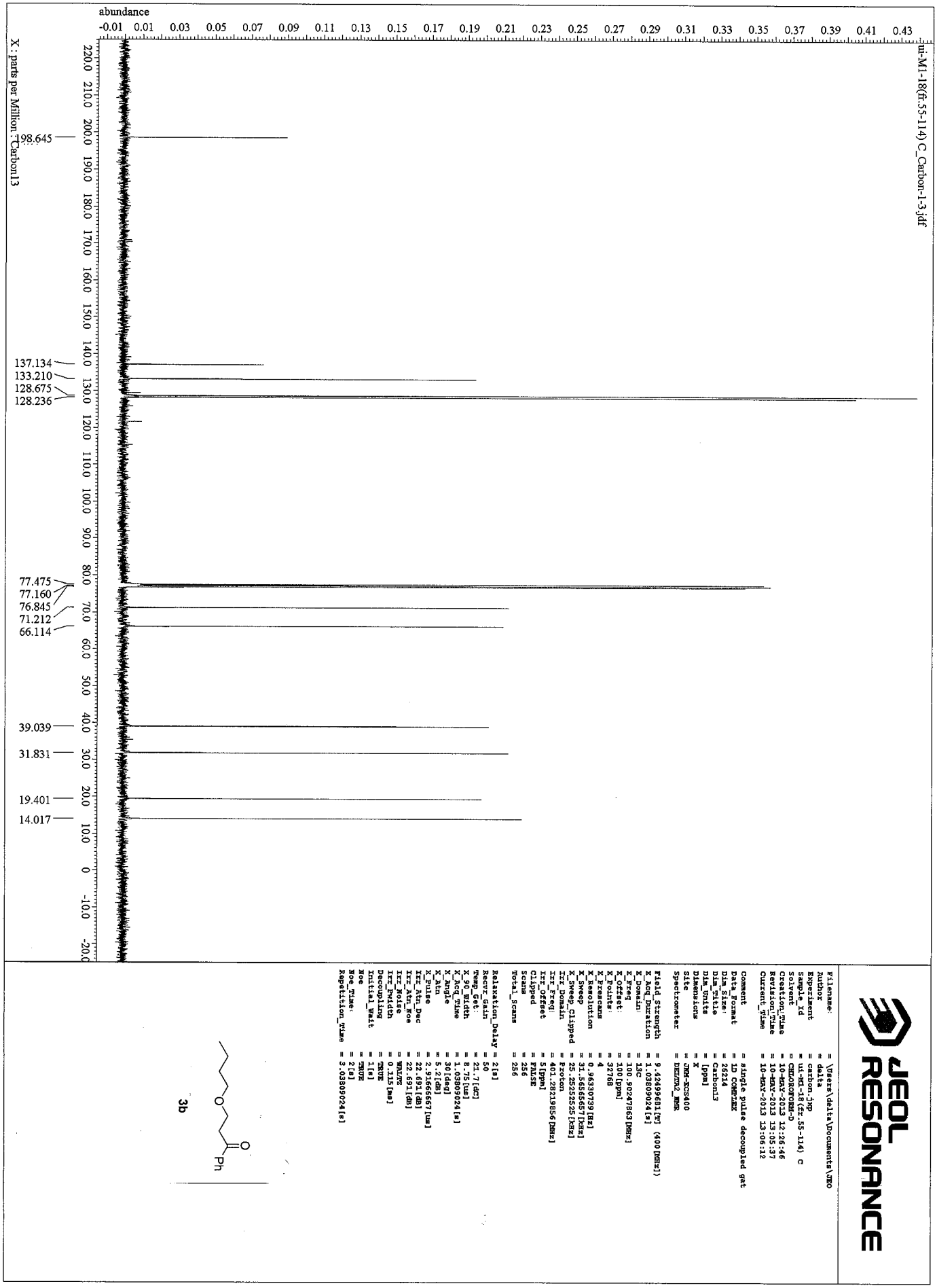
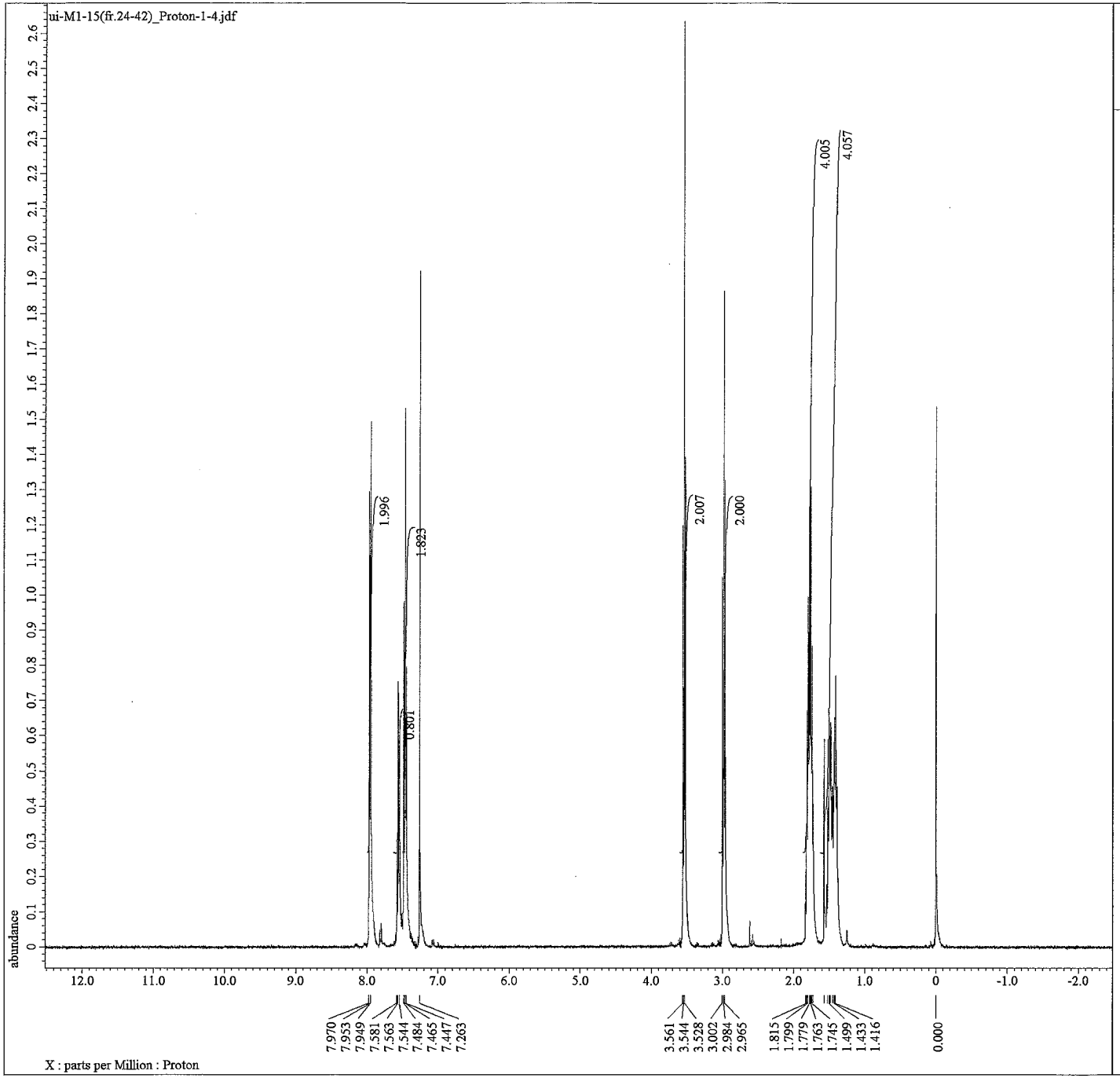
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-M1-18(fr.55-114) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 10-MAY-2013 12:13:05 |
| Revision_Time | = 10-MAY-2013 13:04:13 |
| Current_Time | = 10-MAY-2013 13:04:23 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.1757952[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 48 |
| Temp_Get | = 21.1[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.1757952[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.1757952[s] |




**3b**


abundance
ui-M1-18(ff.55-114) C_Carbon-1-3.jdf
X : parts per Million : Carbon13
198.645
137.134
133.210
128.675
128.236
77.475
77.160
76.845
71.212
66.114
39.039
31.831
19.401
14.017
JEOL RESONANCE
Filename = \Users\delta\Documents\NMR
Author = delta
Experiment = carbon.jxp
Sample_Id = ui-M1-18(ff.55-114) C
Solvent = CHLOROFORM-D
Creation_Time = 10-MAY-2013 12:26:46
Revision_Time = 10-MAY-2013 13:05:37
Current_Time = 10-MAY-2013 13:06:12
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC5400
Spectrometer = DELTA2_NMR
Field_Strength = 9.424996811[T] (400[MHz])
X_Acq_Duration = 1.038090924[s]
X_Domain = 13C
X_Freq = 100.9024763[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.963307399[Hz]
X_Sweep = 31.565656557[kHz]
X_Sweep_Clipped = 25.252525255[kHz]
Irr_Domain = Proton
Irr_Freq = 401.2821986[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recv_Gain = 50
Temp_Get = 21.7[dC]
X_90_Width = 8.75[us]
X_Acq_Time = 1.038090924[s]
X_Angle = 30[deg]
X_Atn = 5.2[dB]
X_Pulse = 2.916666667[us]
Irr_Atn_Dec = 22.69[dB]
Irr_Atn_Noe = 22.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.038090924[s]
3b
O
O
Ph




JEOL RESONANCE

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Filename          = C:\Users\delta\Documents\J
Author            = delta
Experiment        = proton.jxp
Sample_Id         = ui-M1-15(fr.24-42)
Solvent           = CHLOROFORM-D
Creation_Time     = 25-APR-2013 23:48:49
Revision_Time     = 14-MAY-2013 20:23:43
Current_Time      = 14-MAY-2013 20:23:48

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.42499681[T] (400[MHz])
X_Acq_Duration    = 2.1757952[s]
X_Domain          = 1H
X_Freq            = 401.28219856[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45960208[Hz]
X_Sweep           = 7.53012048[kHz]
X_Sweep_Clipped   = 6.02409639[kHz]
Irr_Domain        = Proton
Irr_Freq          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 401.28219856[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 2
Total_Scans       = 2

Relaxation_Delay  = 5[s]
Recvr_Gain        = 46
Temp_Get          = 20.5[dC]
X_90_Width        = 9.25[us]
X_Acq_Time        = 2.1757952[s]
X_Angle           = 45[deg]
X_Atn             = 0.8[dB]
X_Pulse           = 4.625[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.1757952[s]
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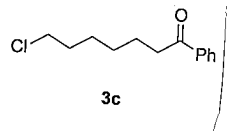
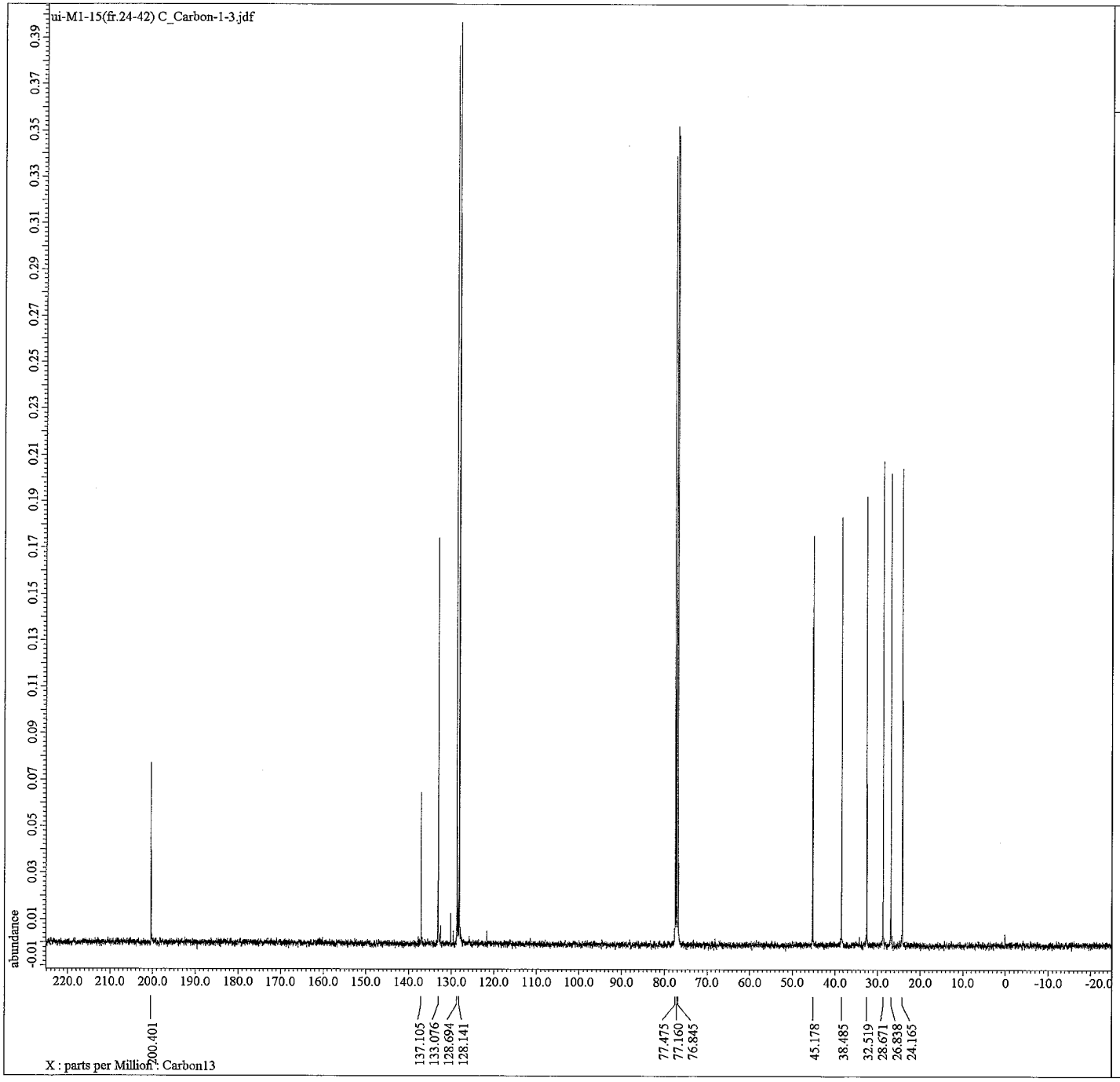



**3c**




JEOL RESONANCE

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| Experiment | = carbon.jxp |
| Sample_Id | = ui-M1-15(fr.24-42) C |
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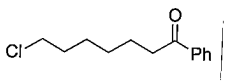
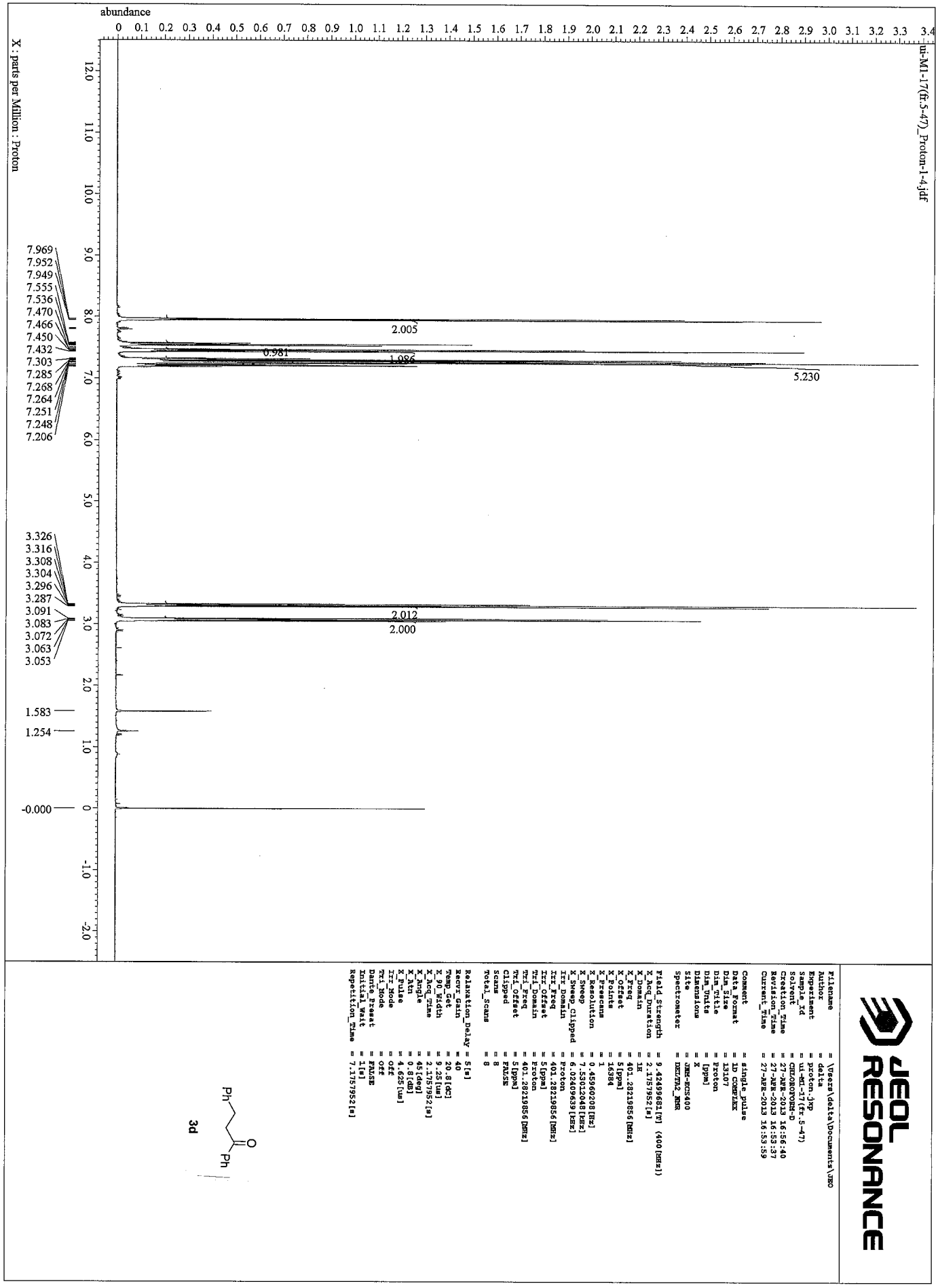
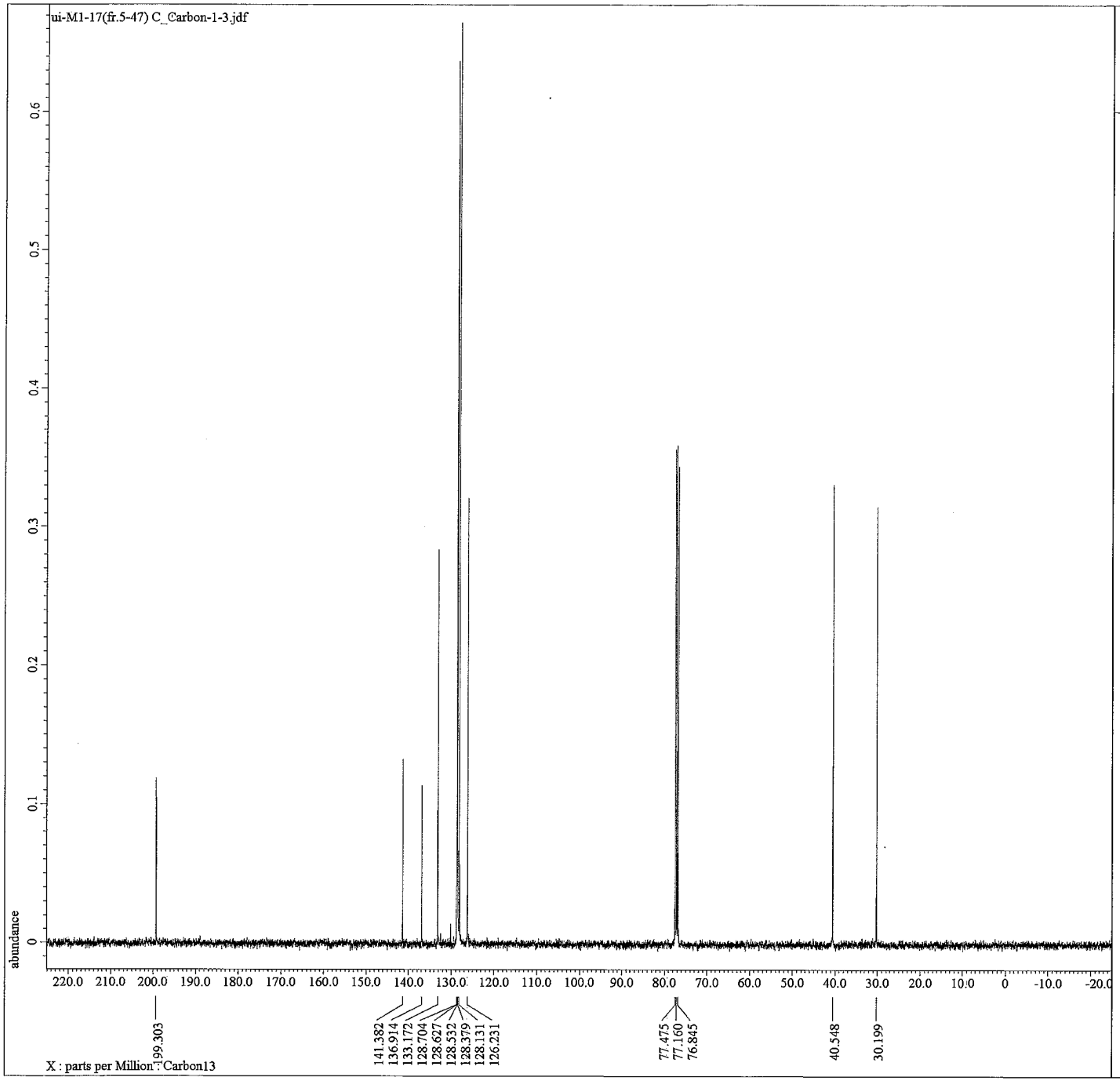
| Revision_Time | = 26-APR-2013 09:57:31 |
| Current_Time | = 26-APR-2013 09:57:35 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.1[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |




**3c**


abundance
X : parts per Million : Proton
ui-M1-17(ff.5-47)_Proton-1-4.jdf
7.969
7.952
7.949
7.555
7.536
7.470
7.466
7.450
7.432
7.303
7.285
7.268
7.264
7.251
7.248
7.206
3.326
3.316
3.308
3.304
3.296
3.287
3.091
3.083
3.072
3.063
3.053
1.583
1.254
-0.000
2.005
0.981
1.086
5.230
2.012
2.000
Filename = \Vesrv\delta\Documents\NEO
Author = delta
Experiment = proton.jxp
Sample_Id = ui-M1-17(ff.5-47)
Solvent = CHLOROFORM-D
Creation_Time = 27-NOV-2013 16:56:40
Revision_Time = 27-NOV-2013 16:53:37
Current_Time = 27-NOV-2013 16:53:59
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681[T] (400[MHz])
X_Acq_Duration = 2.17579952[s]
X_Domain = 1H
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208[Hz]
X_Sweep = 7.53012048[kHz]
X_Sweep_Clipped = 6.02409639[kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 401.28219856[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 20.8[dC]
X_90_Width = 9.25[us]
X_Acq_time = 2.17579952[s]
X_Angle = 45[deg]
X_Atn = 0.8[dB]
X_Pulse = 4.625[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.17579952[s]
Ph
O
Ph
3d




JEOL RESONANCE

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| Creation_Time | = 27-APR-2013 17:01:53 |
| Revision_Time | = 8-MAY-2013 19:54:53 |
| Current_Time | = 8-MAY-2013 19:54:59 |
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| Data_Format | = 1D COMPLEX |
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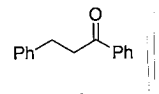
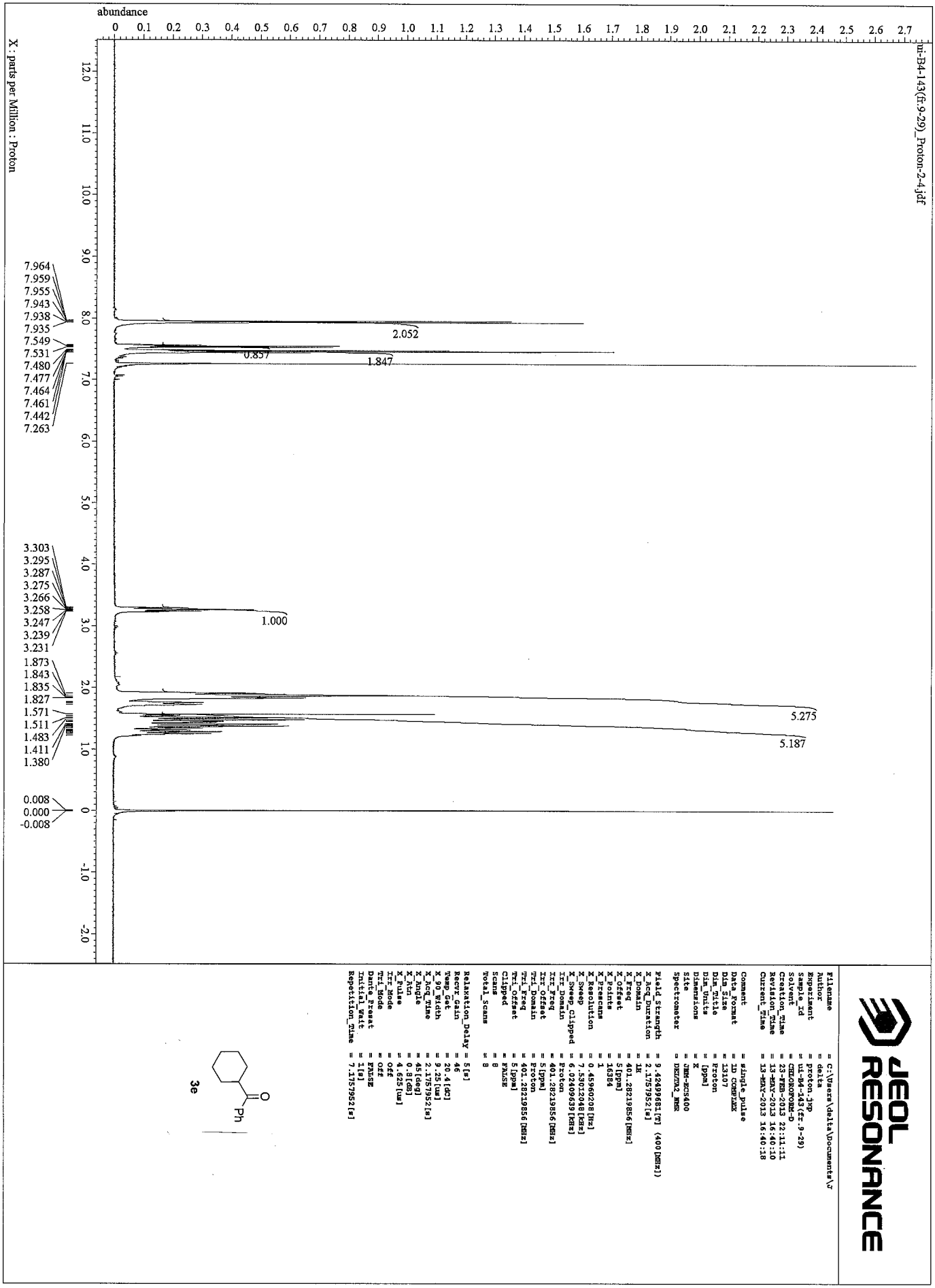
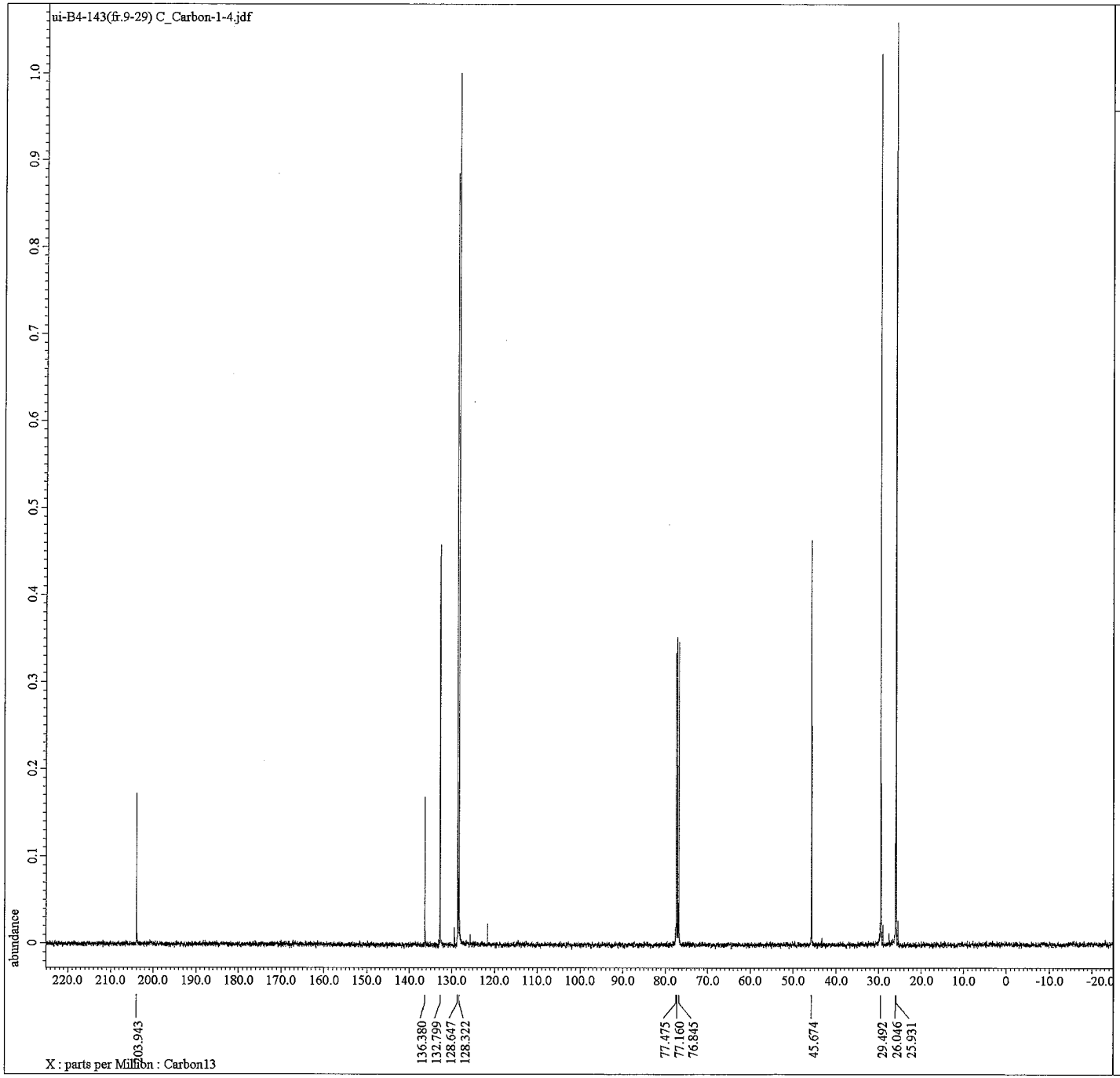
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.9[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |



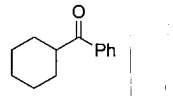

**3d**


abundance
X : parts per Million : Proton
ui-B4-143(fr.9-29)_Proton-2-4.jdf
7.964
7.959
7.955
7.943
7.938
7.935
7.549
7.531
7.480
7.477
7.464
7.461
7.442
7.263
3.303
3.295
3.287
3.275
3.266
3.258
3.247
3.239
3.231
1.873
1.843
1.835
1.827
1.571
1.511
1.483
1.411
1.380
0.008
0.000
-0.008
2.052
0.857
1.847
1.000
5.275
5.187
JEOL RESONANCE
Filename = C:\Users\delta\Documents\J
Author = delta
Experiment = proton.jxp
Sample_id = ui-B4-143(fr.9-29)
Solvent = CHLOROFORM-D
Creation_Time = 13-FEB-2013 22:11:11
Revision_Time = 13-MAY-2013 16:40:10
Current_Time = 13-MAY-2013 16:40:18
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ORB-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499661[T] (400[MHz])
X_Acq_Duration = 2.17579521[s]
X_Domain = 1H
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208[Hz]
X_Sweep = 7.5301204819[kHz]
X_Sweep_Clipped = 6.0240963839[kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 401.28219856[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Set = 20.4[dC]
X_90_Width = 9.25[us]
X_Acq_Time = 2.17579521[s]
X_Angle = 45[deg]
X_Atn = 0.8[dB]
X_Pulse = 4.625[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.17579521[s]
3e
O
Ph

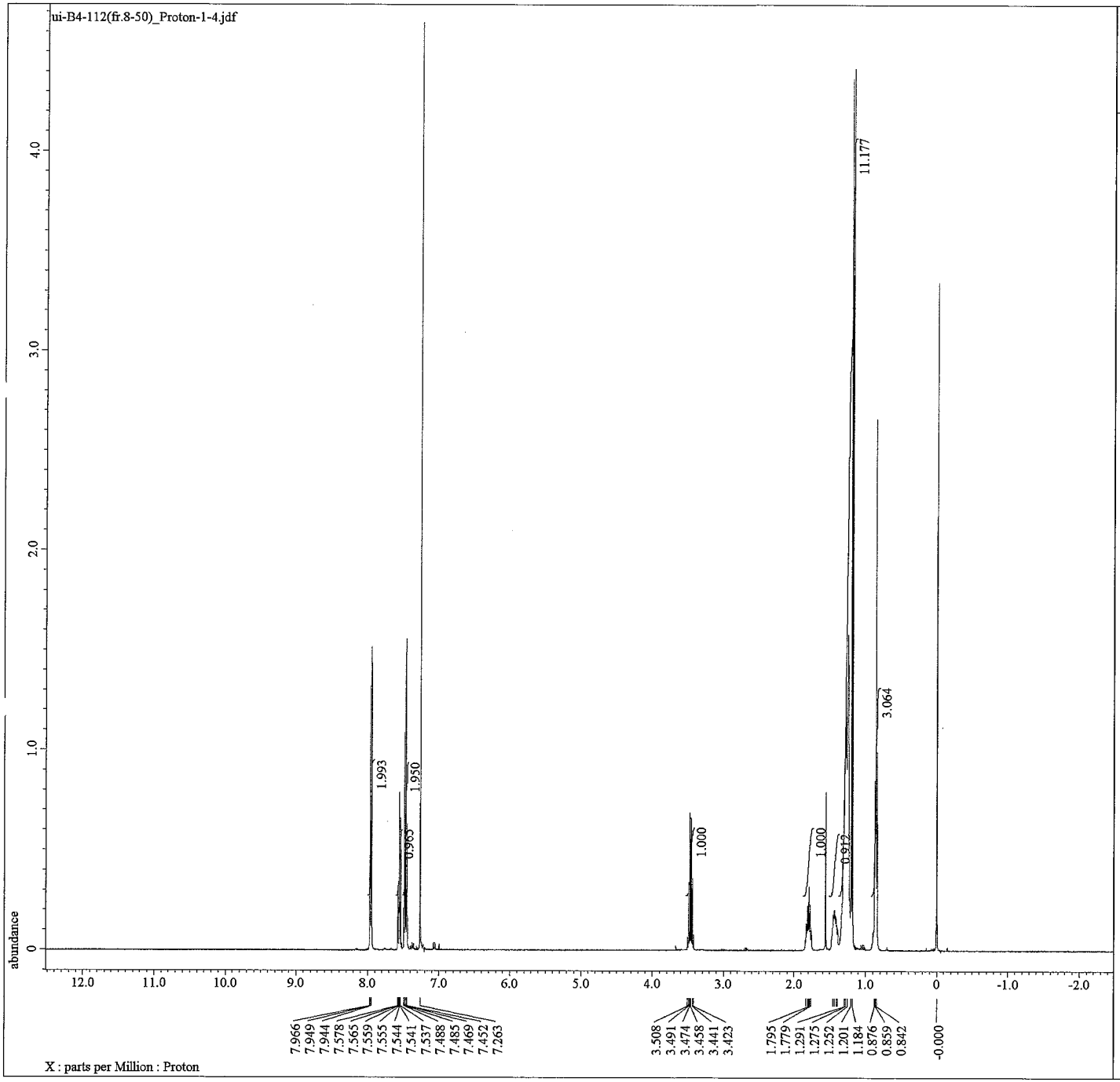



JEOL RESONANCE

| | |
|---|---|
| Filename | = C:\Users\delta\Documents\J |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = ui-B4-143(fr.9-29) C |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 23-FEB-2013 21:42:12 |
| Revision_Time | = 13-MAY-2013 16:40:34 |
| Current_Time | = 13-MAY-2013 16:40:38 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.2[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |

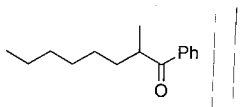



**3e**

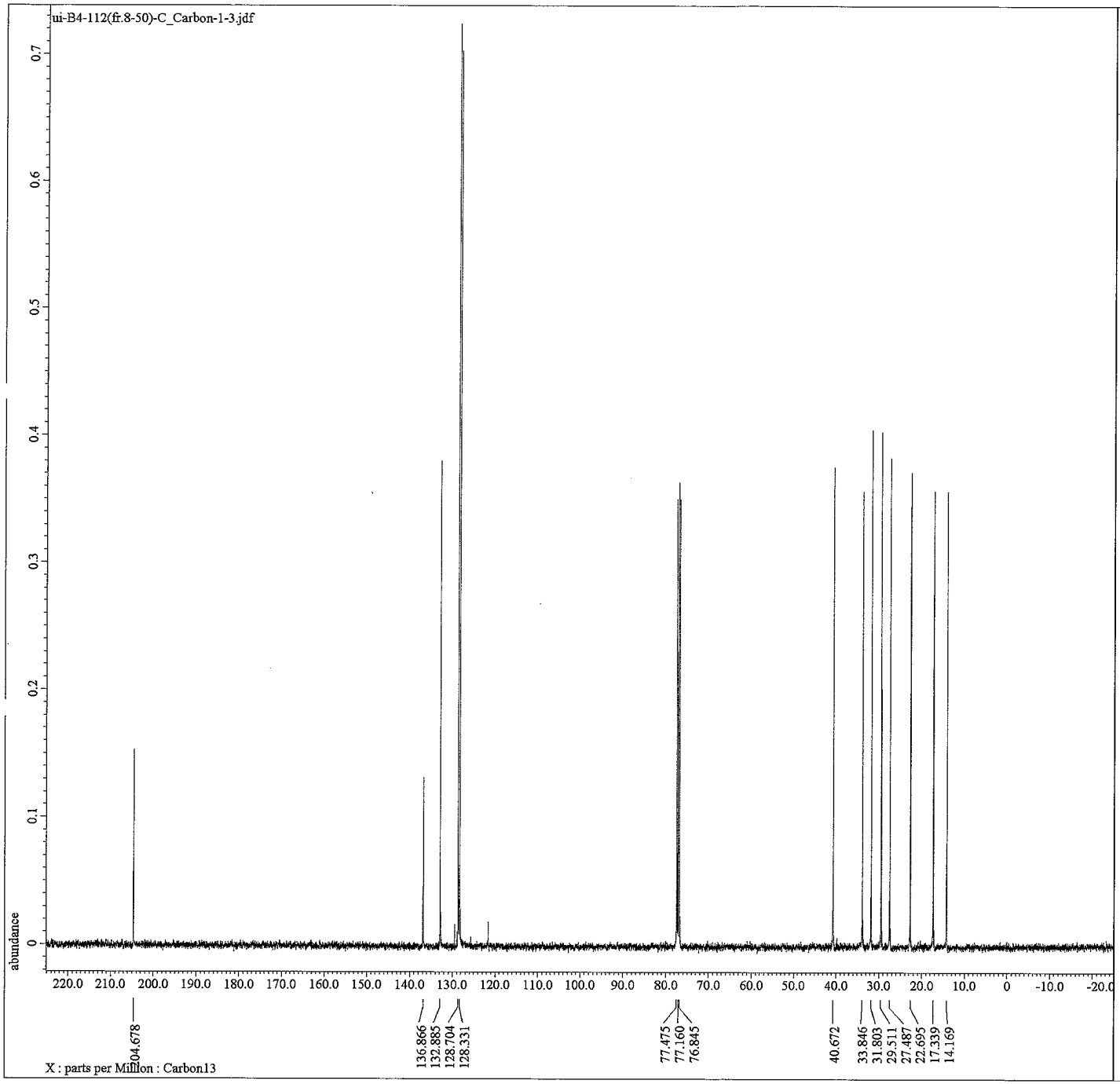



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-B4-112(fr.8-50) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 24-JAN-2013 18:03:03 |
| Revision_Time | = 14-MAR-2013 11:25:19 |
| Current_Time | = 14-MAR-2013 11:25:27 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.1757952[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 16 |
| Total_Scans | = 16 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 48 |
| Temp_Get | = 20.3[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.1757952[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.1757952[s] |

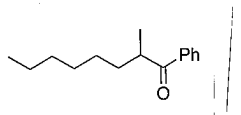



**3f**

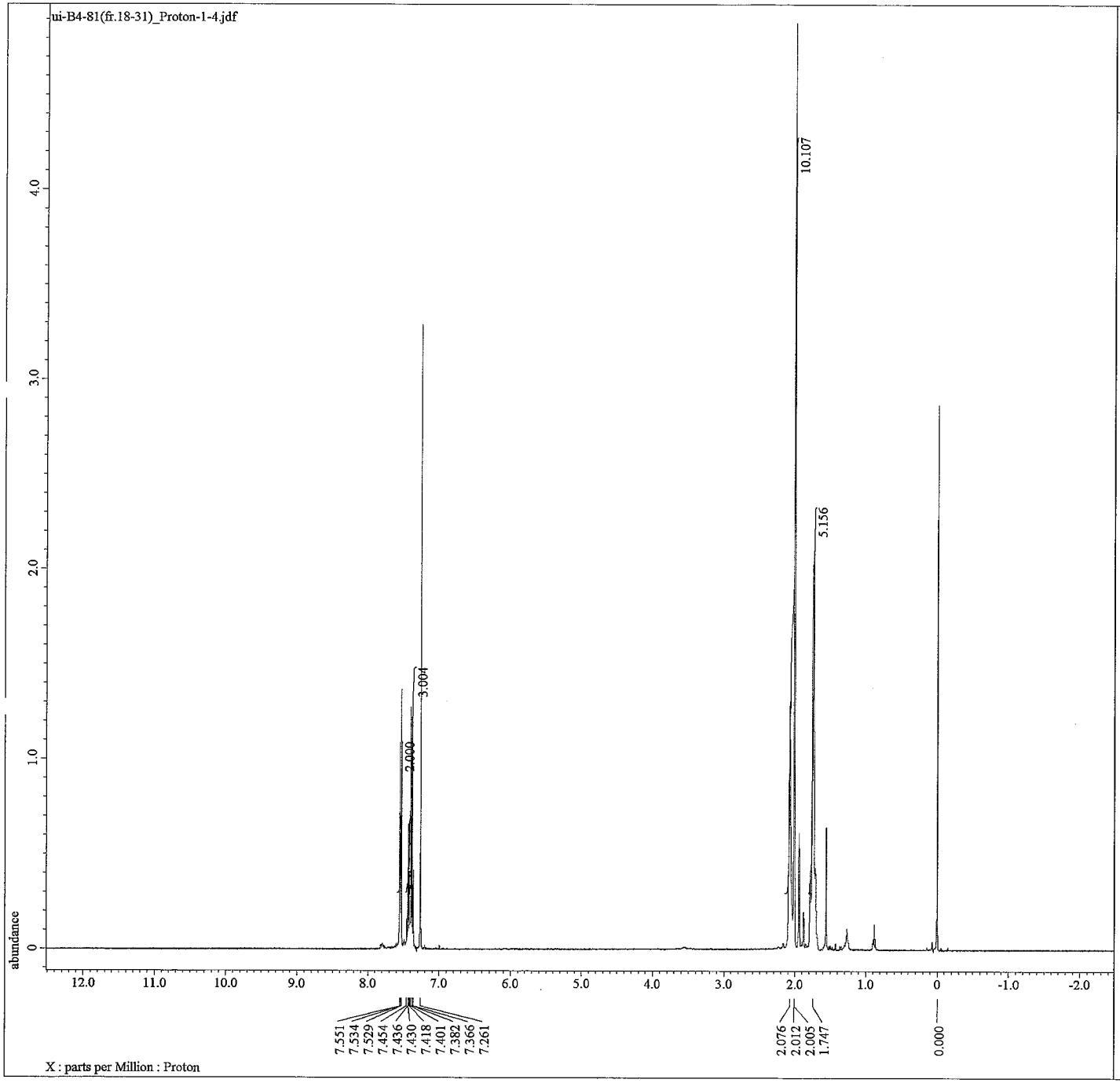



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = ui-B4-112(fr.8-50)-C |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 24-JAN-2013 23:23:05 |
| Revision_Time | = 14-MAR-2013 11:26:13 |
| Current_Time | = 14-MAR-2013 11:26:31 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.5[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |

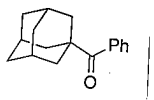



**3f**

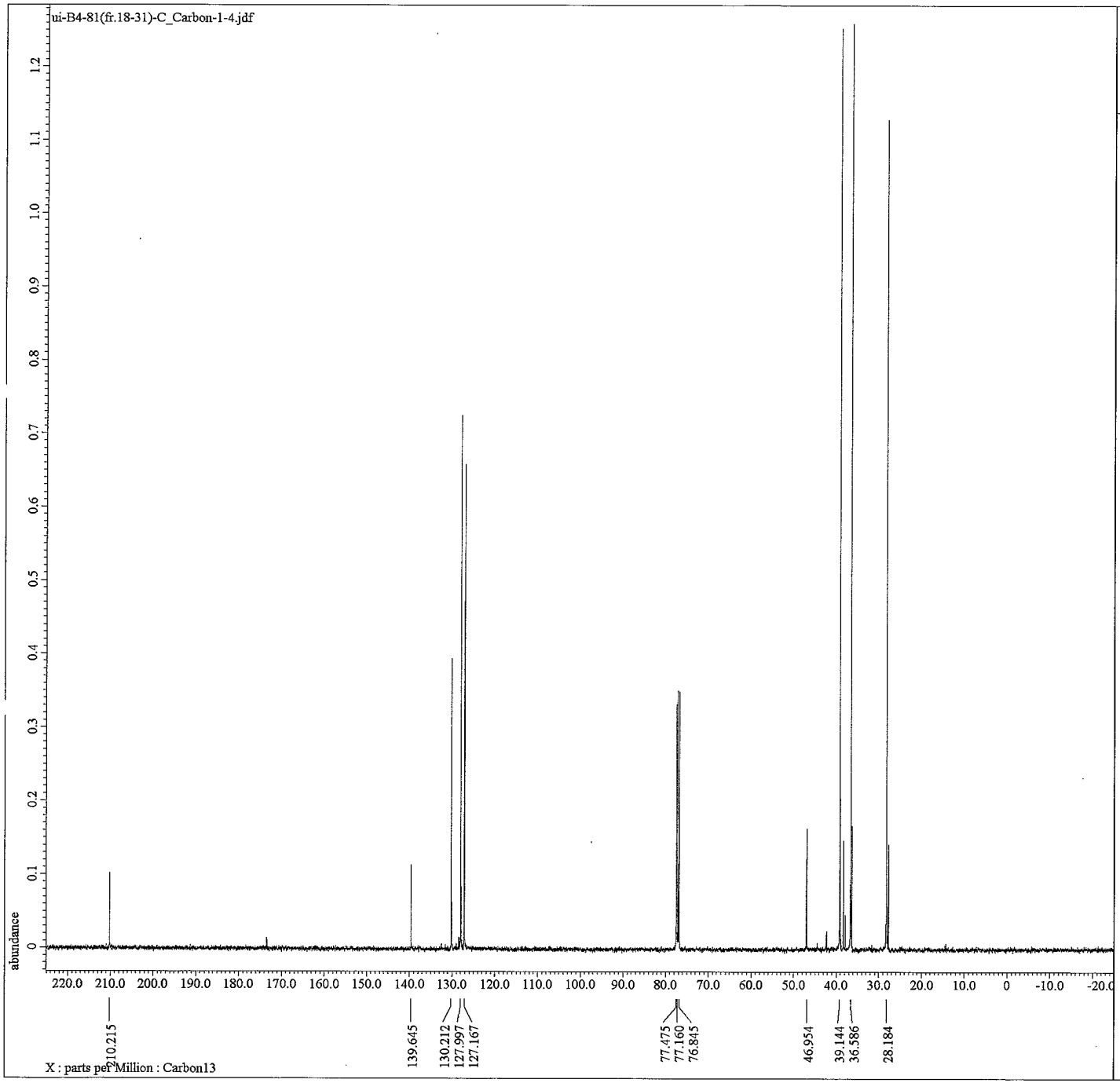



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-B4-81(fr.18-31) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 22-NOV-2012 00:54:39 |
| Revision_Time | = 14-MAR-2013 13:34:35 |
| Current_Time | = 14-MAR-2013 13:34:40 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.1757952[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 48 |
| Temp_Get | = 21[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.1757952[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.1757952[s] |

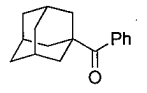



**3g**

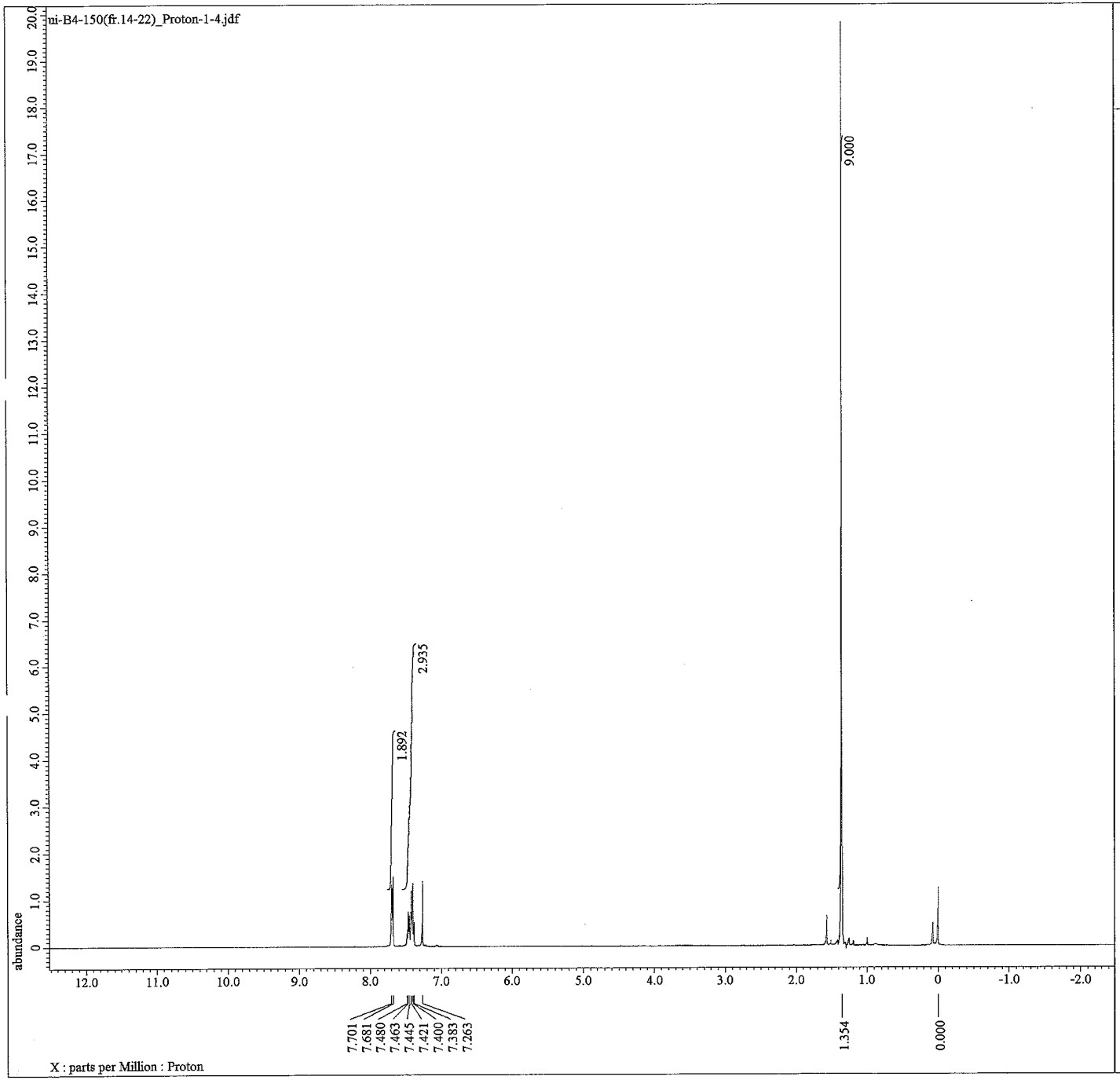



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = ui-B4-81(fr.18-31)-C |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 22-NOV-2012 01:04:35 |
| Revision_Time | = 14-MAR-2013 13:35:36 |
| Current_Time | = 14-MAR-2013 13:35:47 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |

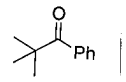



**3g**

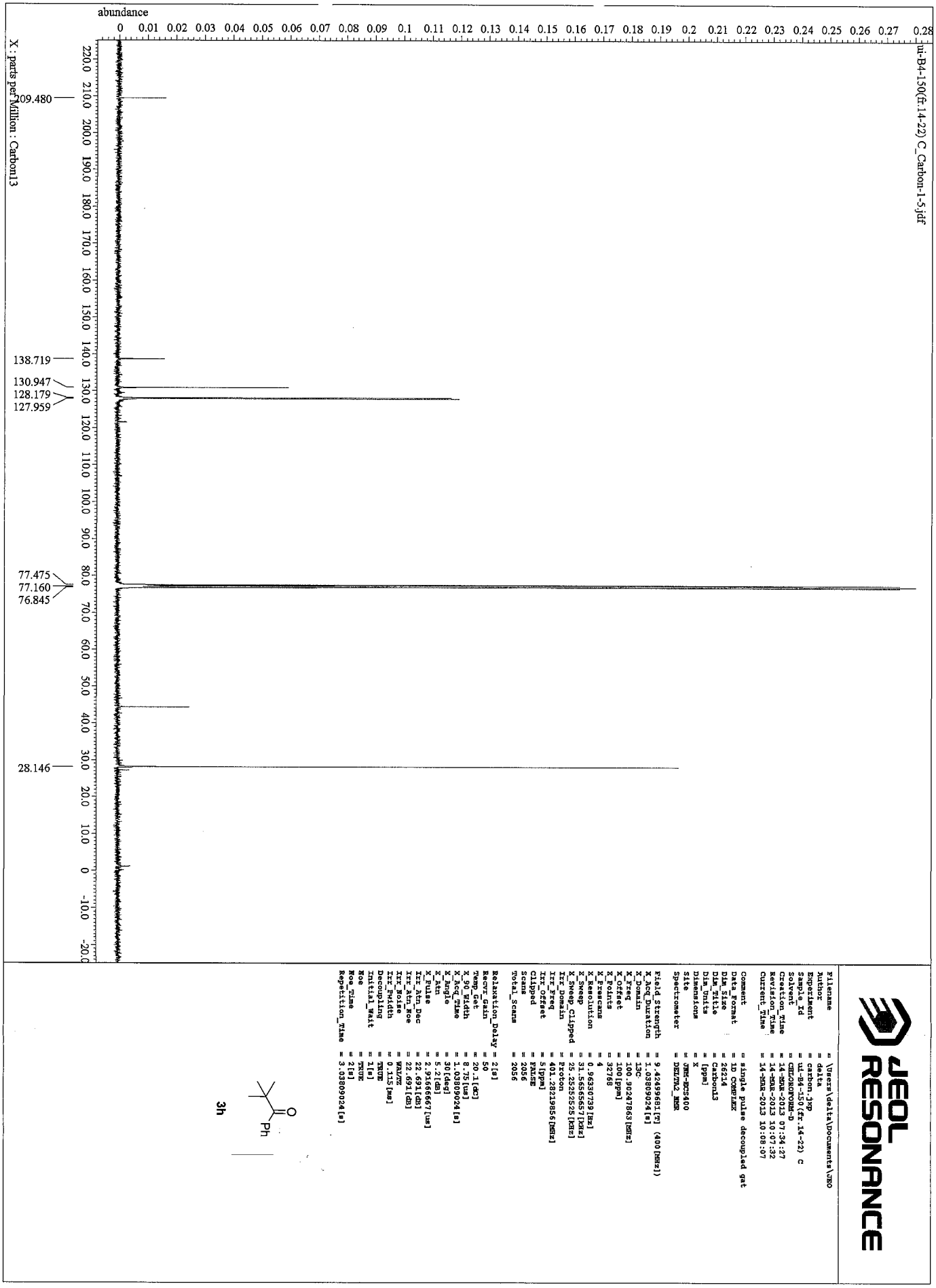


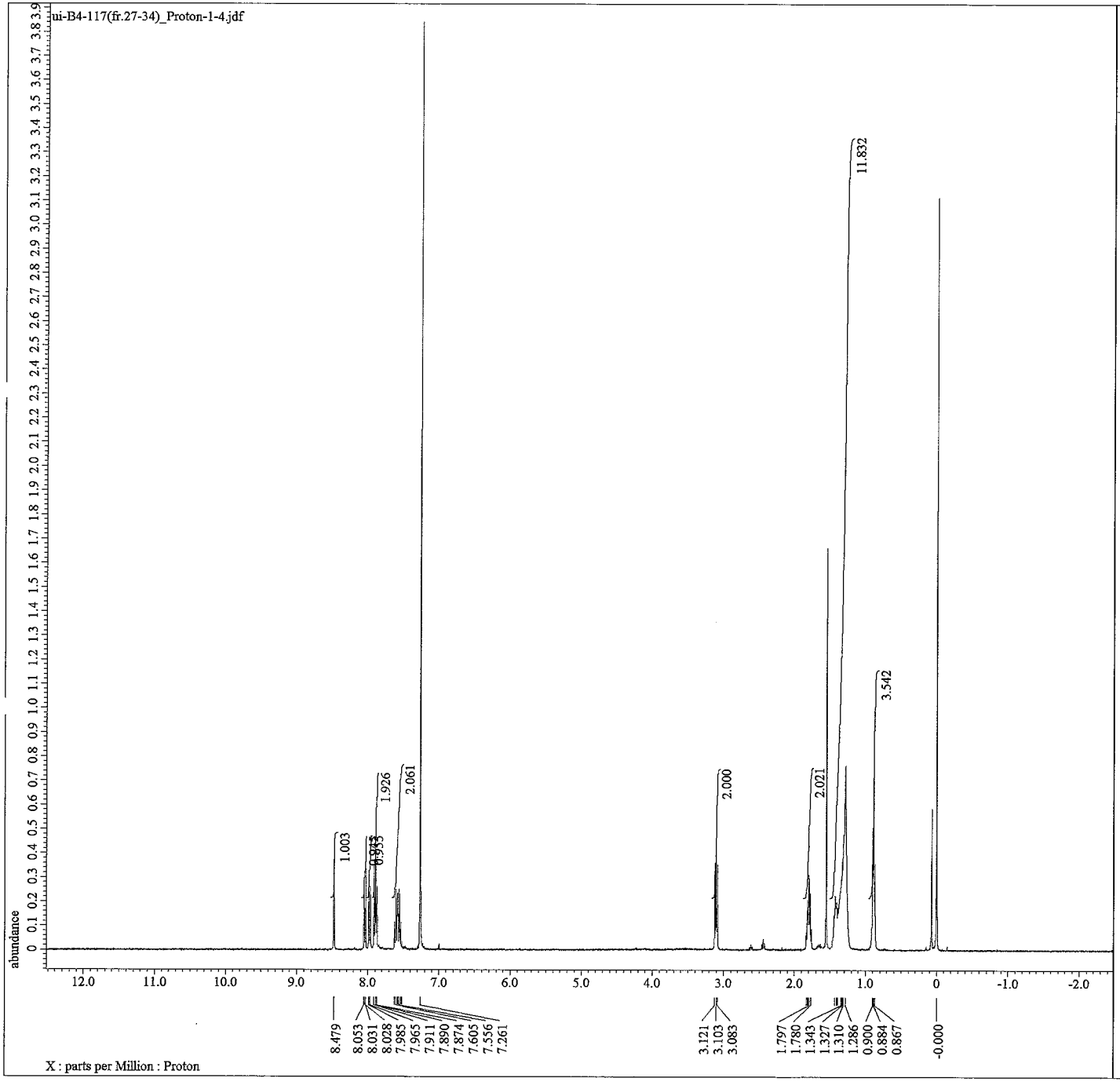

JEOL RESONANCE

```
Filename          = \Users\delta\Documents\JEO
Author            = delta
Experiment        = proton.jxp
Sample_Id         = ui-B4-150(fr.14-22)
Solvent           = CHLOROFORM-D
Creation_Time     = 13-MAR-2013 20:09:08
Revision_Time     = 13-MAR-2013 20:07:03
Current_Time      = 13-MAR-2013 20:07:55

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.42499681[T] (400[MHz])
X_Acq_Duration    = 2.1757952[s]
X_Domain          = 1H
X_Freq            = 401.28219856[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45960208[Hz]
X_Sweep           = 7.53012048[kHz]
X_Sweep_Clipped   = 6.02409639[kHz]
Irr_Domain        = Proton
Irr_Freq          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 401.28219856[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 46
Temp_Get          = 20.3[dC]
X_90_Width        = 9.25[us]
X_Acq_Time        = 2.1757952[s]
X_Angle           = 45[deg]
X_Atn             = 0.8[dB]
X_Pulse           = 4.625[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.1757952[s]
```



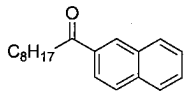

**3h**


abundance
ui-B4-150(ft.14-22) C_Carbon-1-5.jdf
X : parts per Million : Carbon13
209.480
138.719
130.947
128.179
127.959
77.475
77.160
76.845
28.146
JEOL RESONANCE
Filename = \Users\delta\Documents\ORG
Author = delta
Experiment = carbon.jxp
Sample_Id = ui-B4-150(ft.14-22) C
Solvent = CHLOROFORM-D
Creation_Time = 14-MAR-2013 07:34:27
Revision_Time = 14-MAR-2013 10:07:32
Current_Time = 14-MAR-2013 10:08:07
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681[T] (400[MHz])
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.90247863[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 2056
Total_Scans = 2056
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.1[dC]
X_90_Width = 8.75[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 5.2[dB]
X_Pulse = 2.91666667[us]
Irr_Atn_Dec = 22.69[dB]
Irr_Atn_Noe = 22.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.03809024[s]
O
Ph
3h

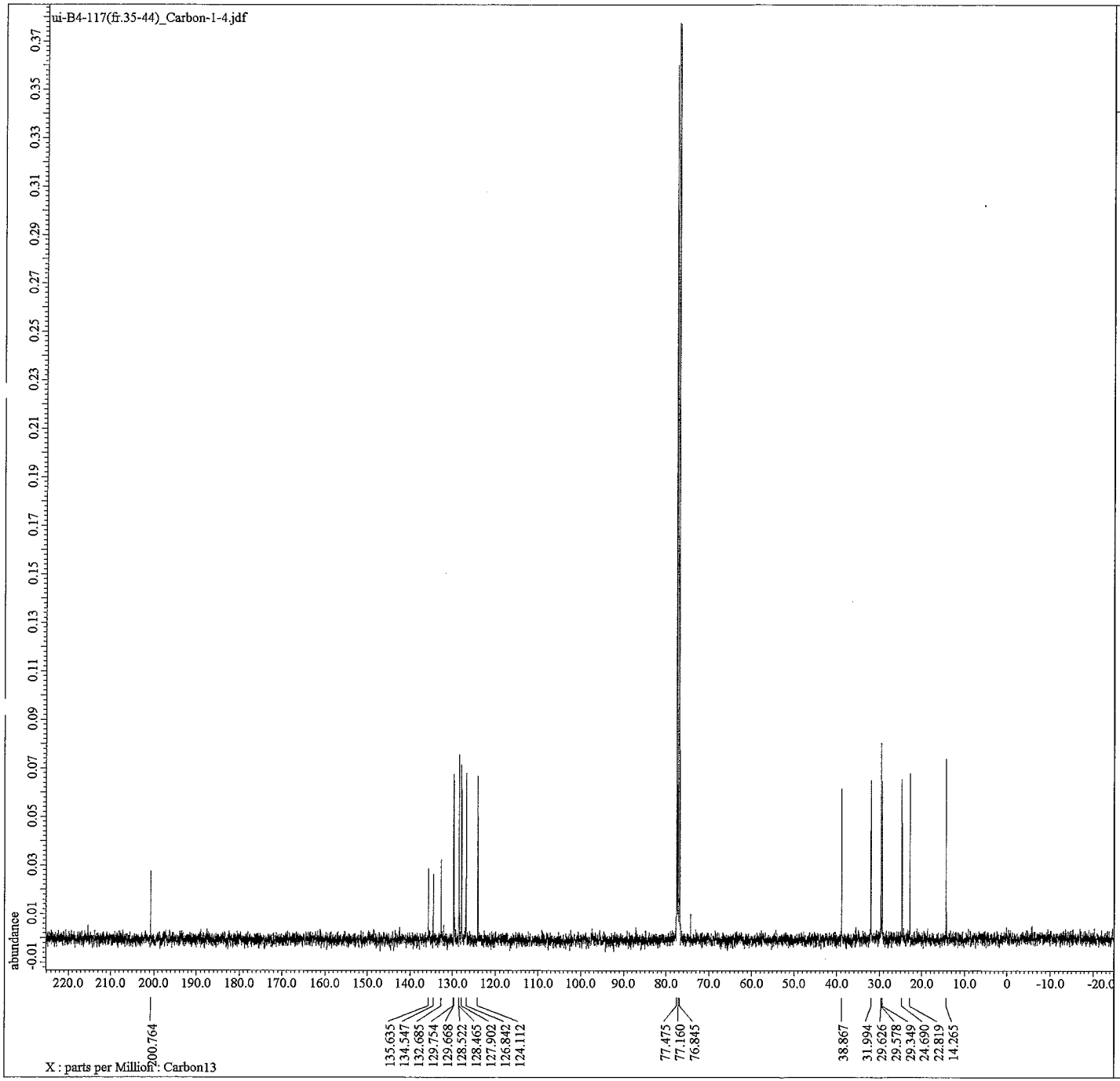



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-B4-117(fr.27-34) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 31-JAN-2013 16:09:45 |
| Revision_Time | = 14-MAR-2013 11:19:45 |
| Current_Time | = 14-MAR-2013 11:19:55 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.1757952[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 16 |
| Total_Scans | = 16 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 52 |
| Temp_Get | = 20[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.1757952[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.1757952[s] |

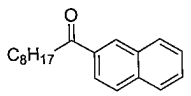



**3i**

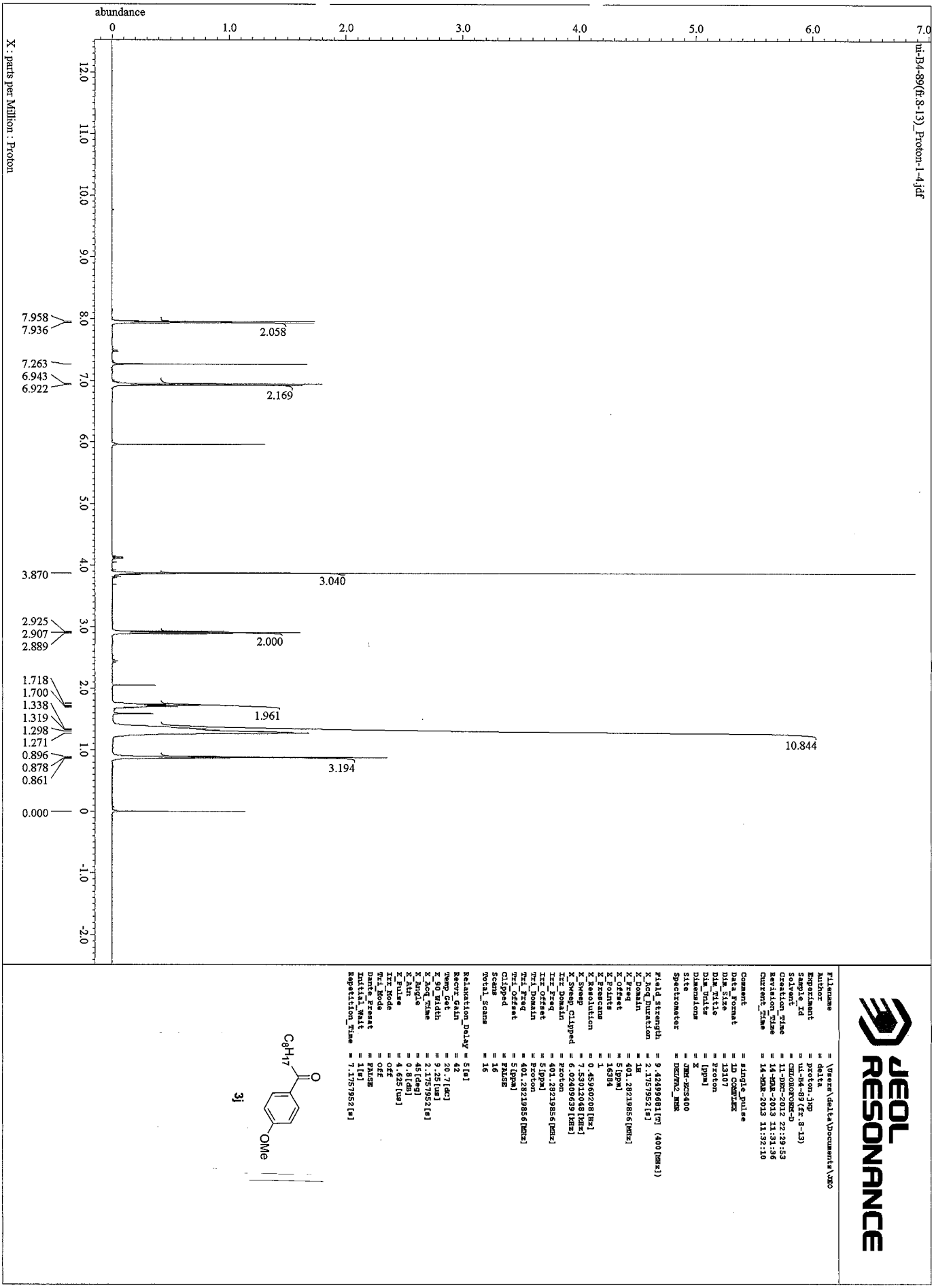


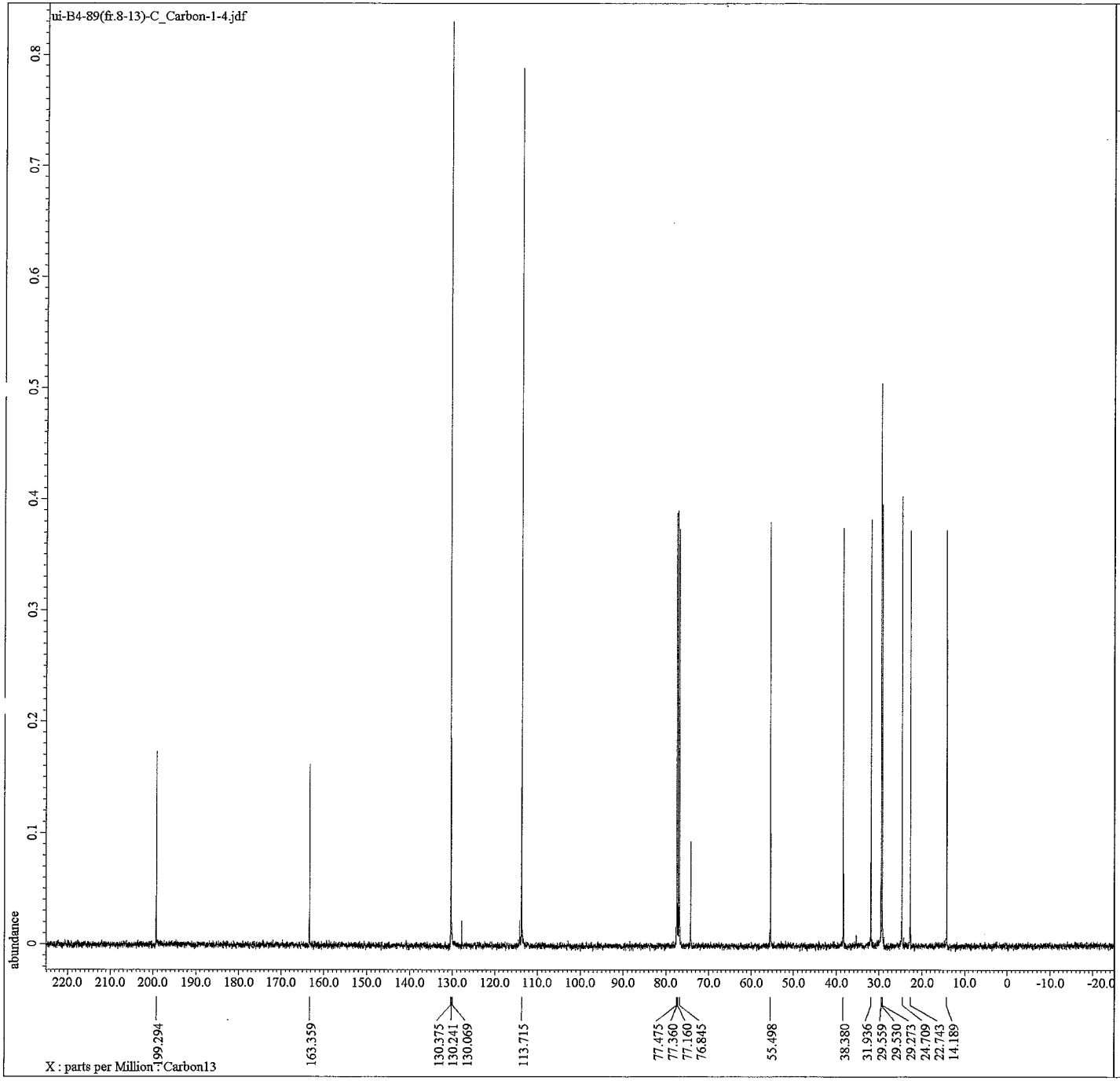

JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = ui-B4-117(fr.35-44) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 31-JAN-2013 18:07:05 |
| Revision_Time | = 14-MAR-2013 11:13:32 |
| Current_Time | = 14-MAR-2013 11:13:53 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.3[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |



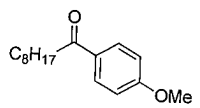

**3i**


abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
ui-B4-89(ft.8-13)_Proton-1-4.jdf
X : parts per Million : Proton
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.958
7.936
2.058
7.263
6.943
6.922
2.169
3.870
3.040
2.925
2.907
2.889
2.000
1.718
1.700
1.338
1.319
1.298
1.271
1.961
10.844
0.896
0.878
0.861
3.194
0.000
Filename = \Users\delta\Documents\XEO
Author = delta
Experiment = proton.jxp
Sample_Id = ui-B4-89(ft.8-13)
Solvent = CHLOROFORM-D
Creation_Time = 11-DEC-2012 22:29:53
Revision_Time = 14-MAR-2013 11:31:36
Current_Time = 14-MAR-2013 11:32:10
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.424996811[T] (400[MHz])
X_Acq_Duration = 2.17579521[s]
X_Domain = 1H
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208[Hz]
X_Sweep = 7.53012048[kHz]
X_Sweep_Clipped = 6.02409639[kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 401.28219856[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 20.7[dC]
X_90_Width = 9.25[us]
X_Acq_Time = 2.17579521[s]
X_Angle = 45[deg]
X_Atn = 0.8[dB]
X_Pulse = 4.625[us]
Irr_Mode = off
Tri_Mode = off
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.17579521[s]
C8H17
O
OMe
3j

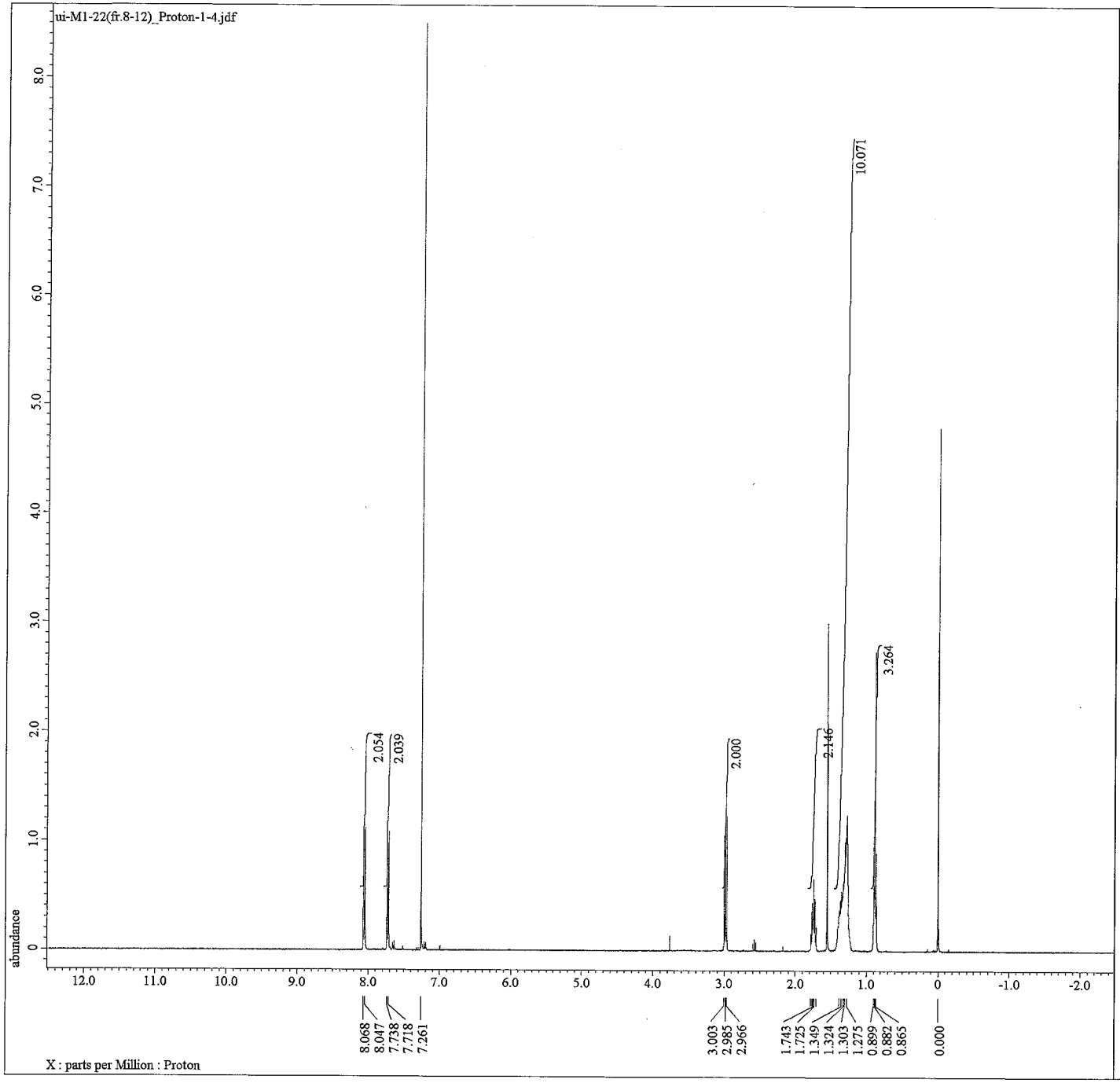



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = ui-B4-89(fr.8-13)-C |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 12-DEC-2012 10:14:05 |
| Revision_Time | = 14-MAR-2013 11:33:31 |
| Current_Time | = 14-MAR-2013 11:34:06 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |

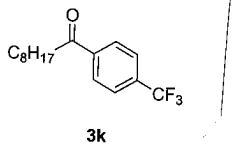



**3j**

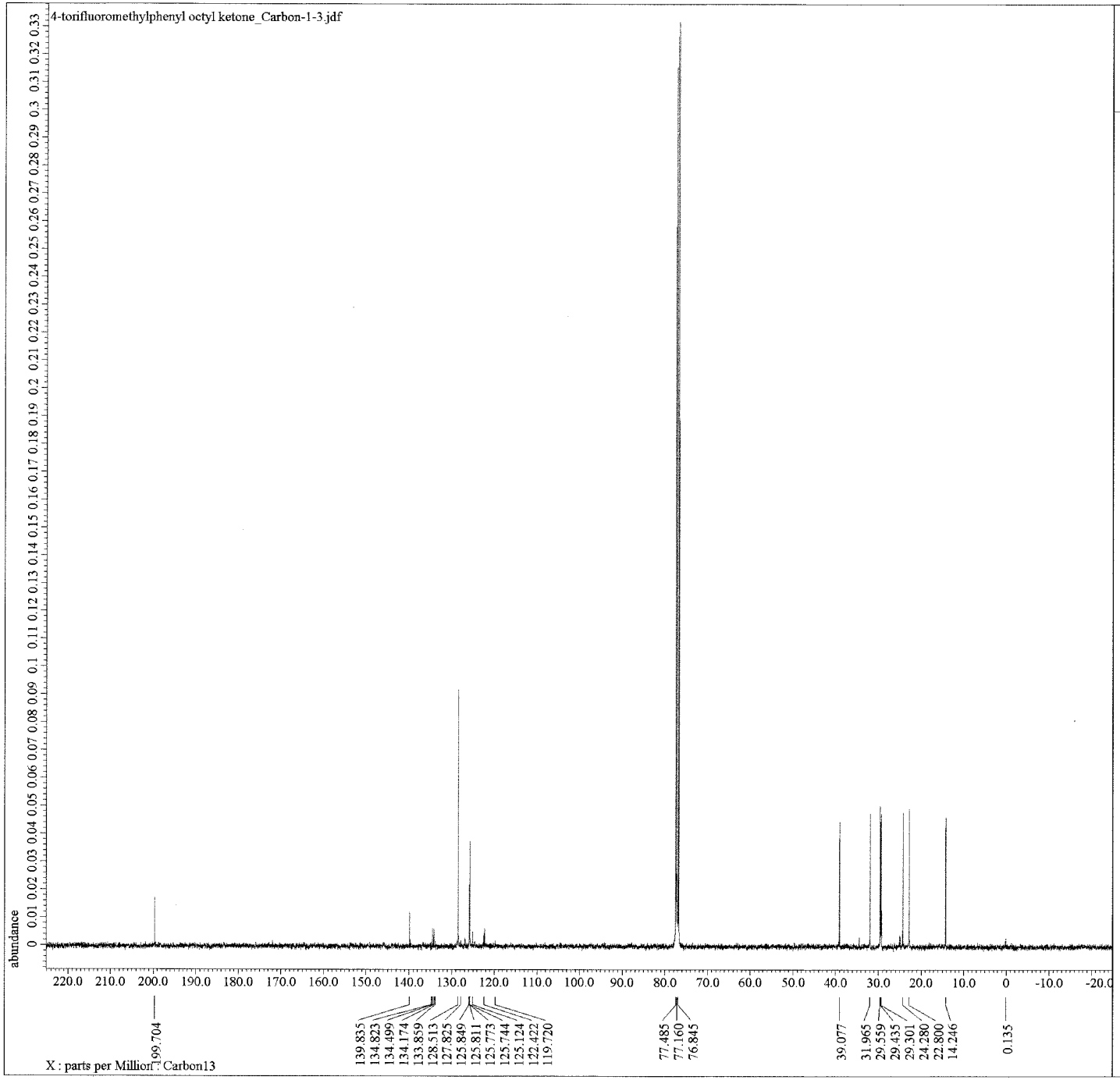



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-M1-22(fr.8-12) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 10-MAY-2013 23:25:37 |
| Revision_Time | = 11-MAY-2013 00:42:14 |
| Current_Time | = 11-MAY-2013 00:42:28 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.1757952[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.3[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.1757952[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.1757952[s] |

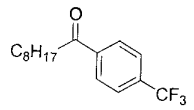



**3k**

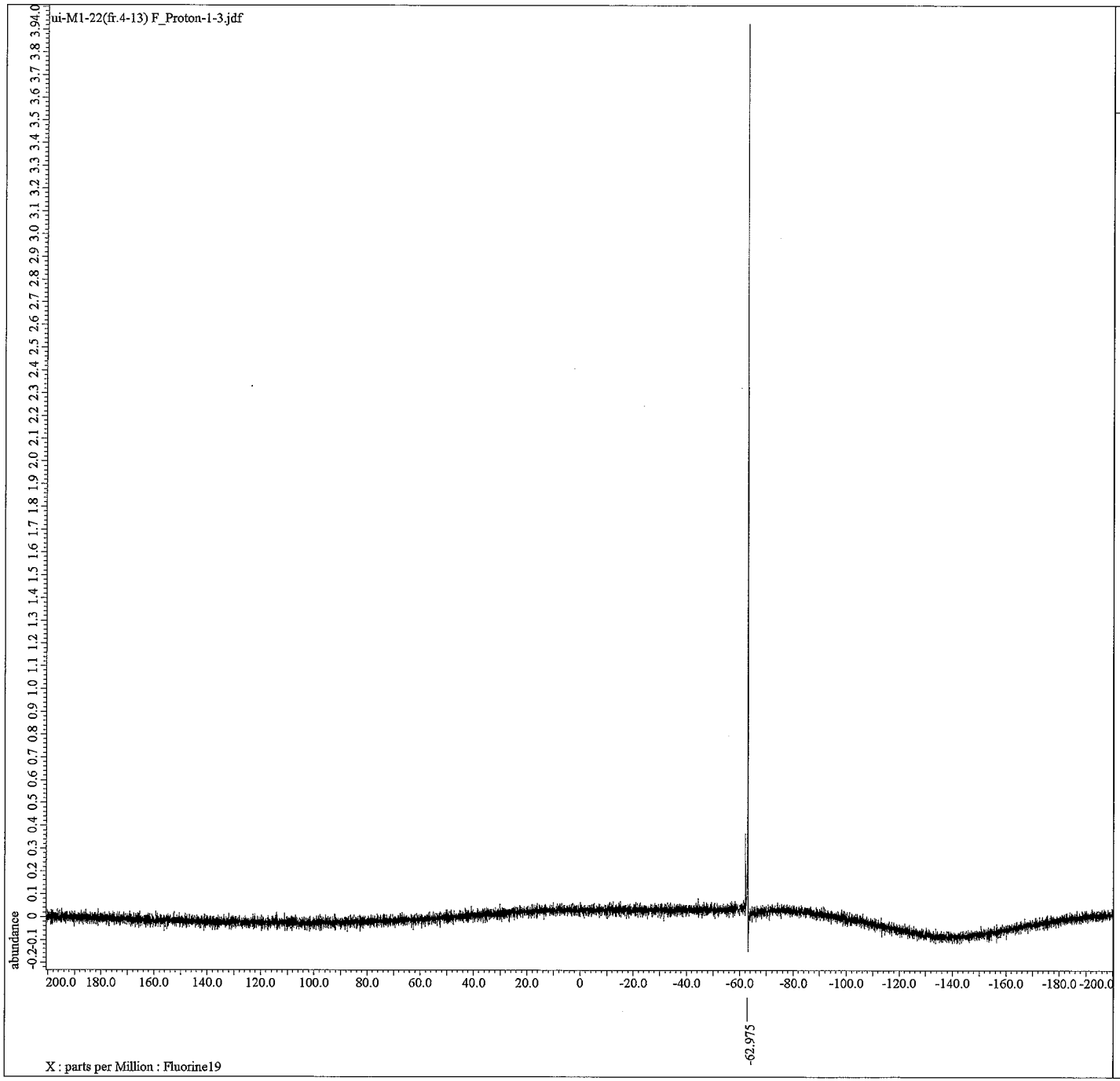



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = 4-torifluoromethylphenyl o |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 15-MAY-2013 11:49:21 |
| Revision_Time | = 15-MAY-2013 14:25:56 |
| Current_Time | = 15-MAY-2013 14:26:26 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JEM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 2048 |
| Total_Scans | = 2048 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.1[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |

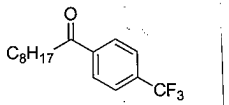



**3k**

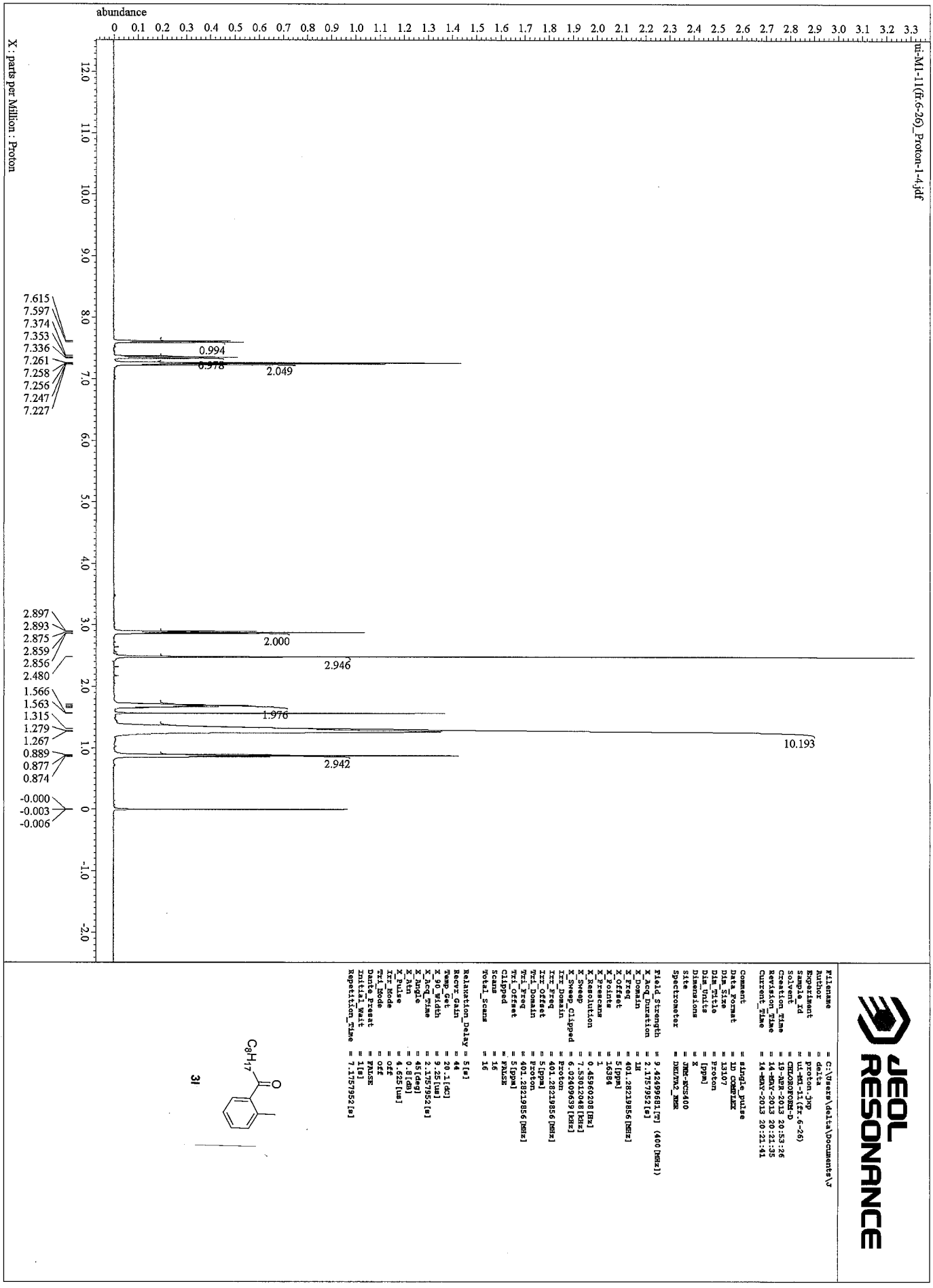


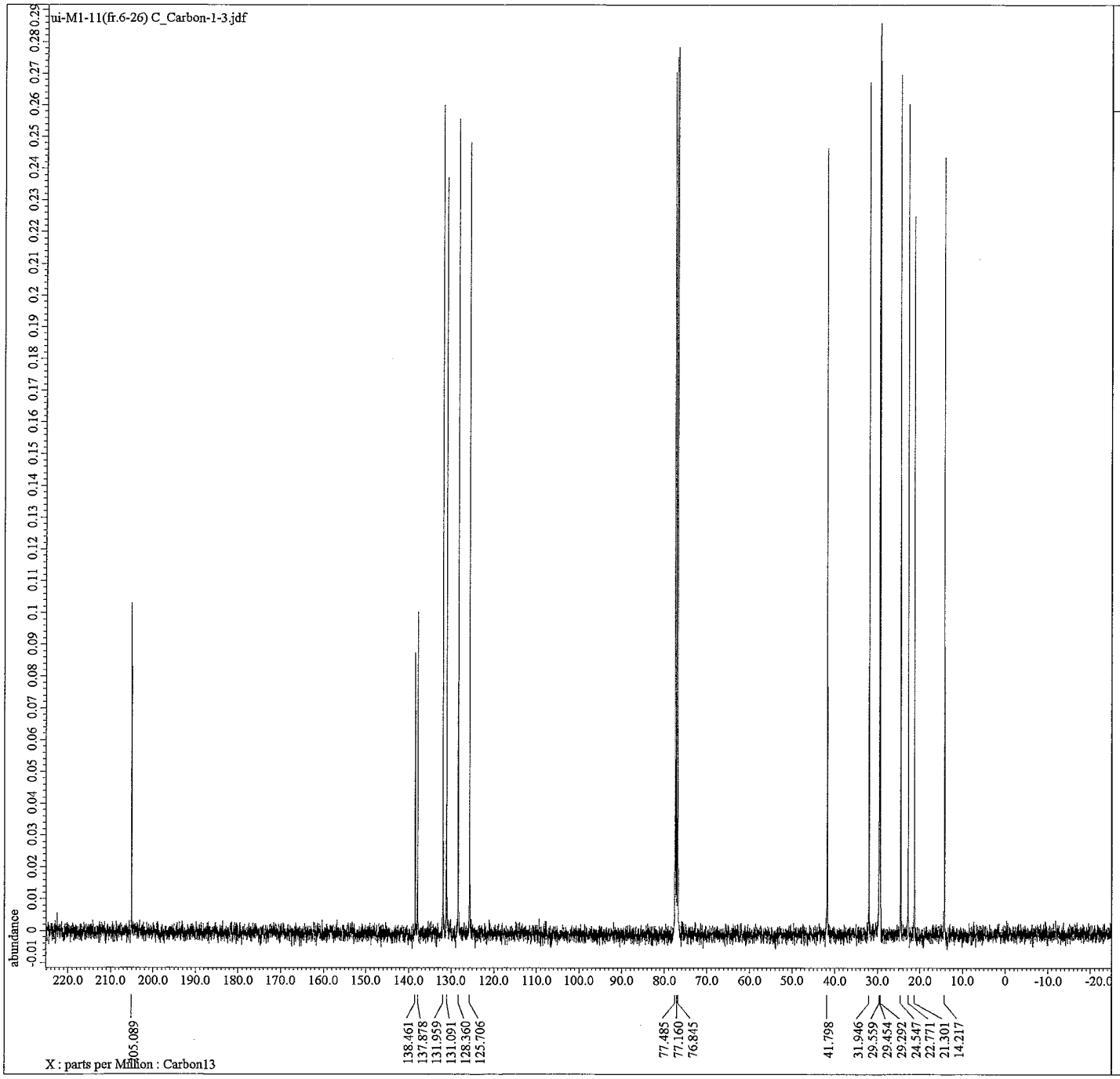

JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-M1-22(fr.4-13) F |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 13-MAY-2013 16:29:48 |
| Revision_Time | = 13-MAY-2013 16:25:50 |
| Current_Time | = 13-MAY-2013 16:26:06 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Fluorine19 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 86.50752[ms] |
| X_Domain | = 19F |
| X_Freq | = 377.58246406[MHz] |
| X_Offset | = 0[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 11.55968868[Hz] |
| X_Sweep | = 189.39393939[kHz] |
| X_Sweep_Clipped | = 151.51515152[kHz] |
| Irr_Domain | = Fluorine19 |
| Irr_Freq | = 377.58246406[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Fluorine19 |
| Tri_Freq | = 377.58246406[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.9[dC] |
| X_90_Width | = 10.75[us] |
| X_Acq_Time | = 86.50752[ms] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 5.375[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 5.08650752[s] |



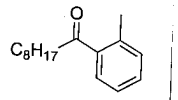

**3k**


abundance
X : parts per Million : Proton
ui-M1-1(fr.6-26)_Proton-1-4.jdf
7.615
7.597
7.374
7.353
7.336
7.261
7.258
7.256
7.247
7.227
0.994
0.978
2.049
2.897
2.893
2.875
2.859
2.856
2.480
2.000
2.946
1.566
1.563
1.315
1.279
1.267
0.889
0.877
0.874
1.976
10.193
2.942
-0.000
-0.003
-0.006
Filename = C:\Users\delta\Documents\J
Author = delta
Experiment = proton.jxp
Sample_Id = ui-M1-1(fr.6-26)
Solvent = CHLOROFORM-D
Creation_Time = 19-APR-2013 20:53:26
Revision_Time = 14-MAY-2013 20:21:35
Current_Time = 14-MAY-2013 20:21:41
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.4249968[T] (400[MHz])
X_Acq_Duration = 2.1757952[s]
X_Domain = 1H
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208[Hz]
X_Sweep = 7.53012048[kHz]
X_Sweep_Clipped = 6.02409639[kHz]
X_Units = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Irr_Domain = Proton
Mpi_Freq = 401.28219856[MHz]
Mpi_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 20.1[dC]
X_90_Width = 9.25[us]
X_Acq_Time = 2.1757952[s]
X_Angle = 45[deg]
X_Atten = 0.0[dB]
X_Pulse = 4.62[us]
Irr_Mode = off
Mpi_Mode = off
Decpl_Present = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.1757952[s]
JEOL RESONANCE
3l
C8H17
O

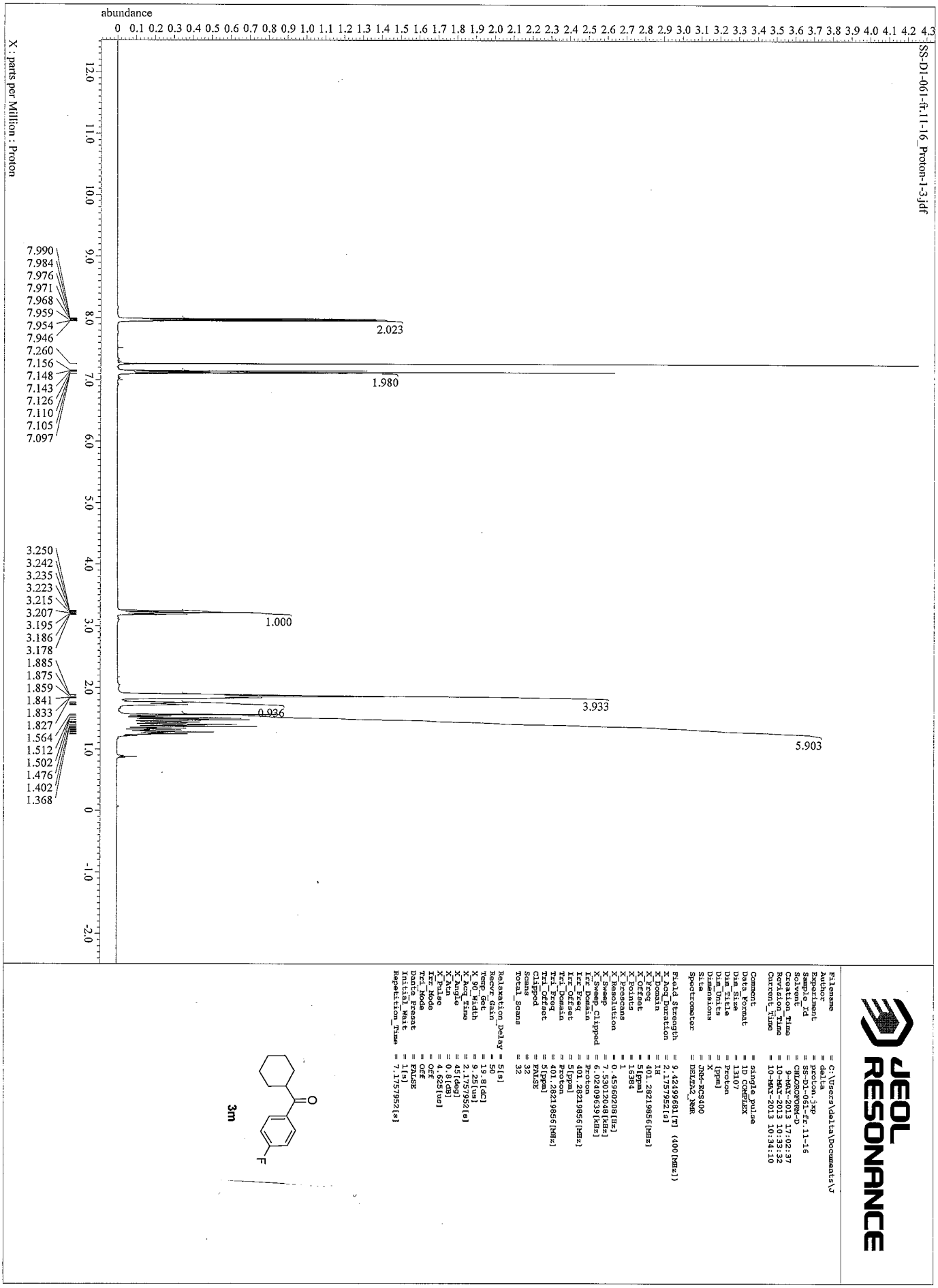


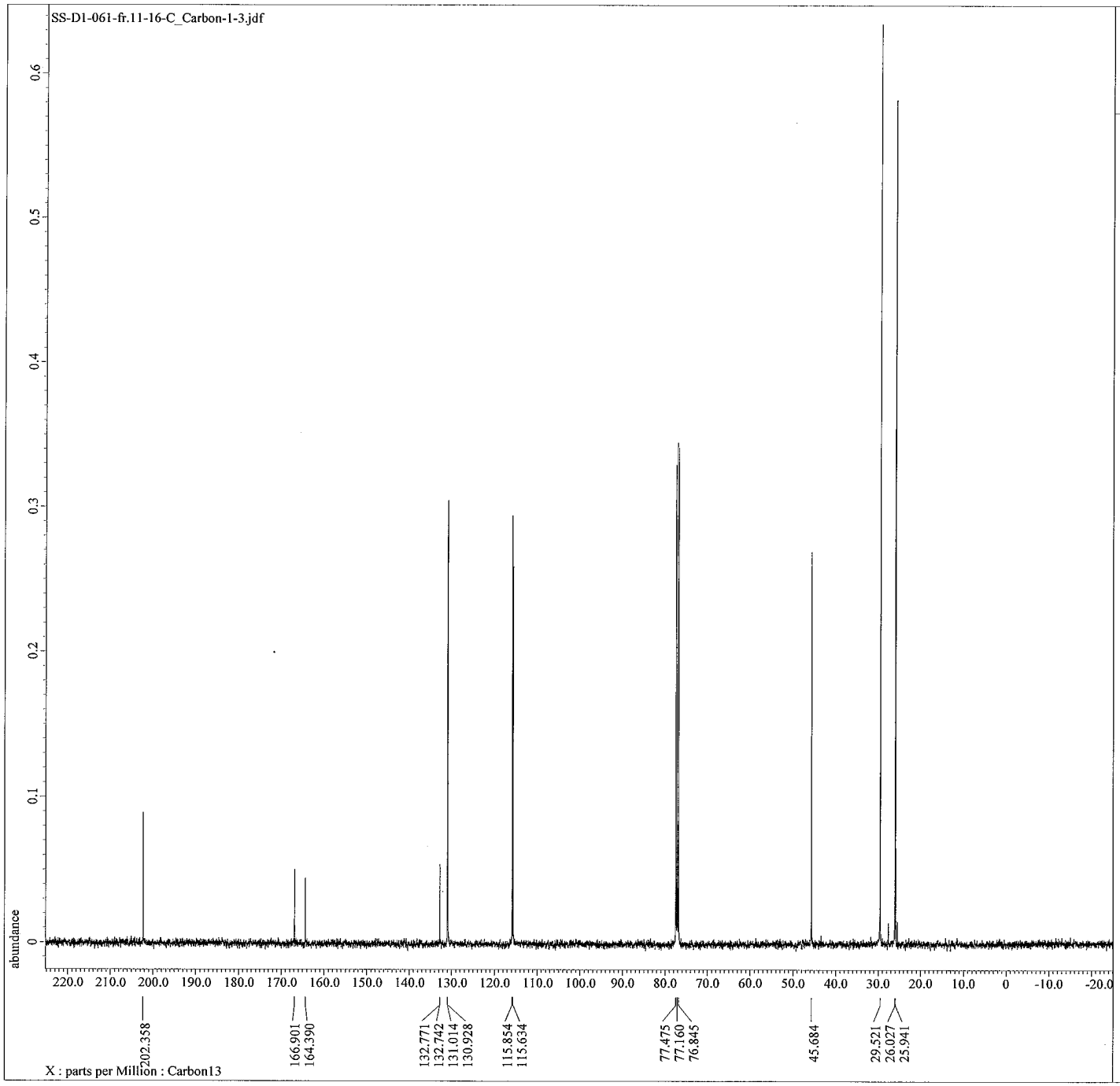

JEOL RESONANCE

```
Filename          = C:\Users\delta\Documents\J
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = ui-M1-11(fr.6-26) C
Solvent           = CHLOROFORM-D
Creation_Time     = 19-APR-2013 21:06:14
Revision_Time     = 14-MAY-2013 20:20:23
Current_Time      = 14-MAY-2013 20:20:27

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.42499681[T] (400[MHz])
X_Acq_Duration    = 1.03809024[s]
X_Domain          = 13C
X_Freq            = 100.90247863[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.96330739[Hz]
X_Sweep           = 31.56565657[kHz]
X_Sweep_Clipped   = 25.25252525[kHz]
Irr_Domain        = Proton
Irr_Freq          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 20.7[dC]
X_90_Width        = 8.75[us]
X_Acq_Time        = 1.03809024[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 2.91666667[us]
Irr_Atn_Dec       = 22.691[dB]
Irr_Atn_Noe       = 22.691[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.03809024[s]
```



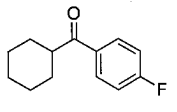

**3l**


abundance
SS-D1-061-fr.11-16_Proton-1-3.jdf
X : parts per Million : Proton
7.990
7.984
7.976
7.971
7.968
7.959
7.954
7.946
7.260
7.156
7.148
7.143
7.126
7.110
7.105
7.097
3.250
3.242
3.235
3.223
3.215
3.207
3.195
3.186
3.178
1.885
1.875
1.859
1.841
1.833
1.827
1.564
1.512
1.502
1.476
1.402
1.368
2.023
1.980
1.000
3.933
0.936
5.903
3m
O
F
JEOL RESONANCE
Filename = C:\Users\delta\Documents\J
Author = delta
Experiment = proton.jxp
Sample_Id = SS-D1-061-fr. 11-16
Solvent = CHLOROFORM-D
Creation_Time = 9-MAY-2013 17:02:37
Revision_Time = 10-MAY-2013 10:33:32
Current_Time = 10-MAY-2013 10:34:10
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681[T] (400[MHz])
X_Acq_Duration = 2.17579952[s]
X_Domain = 1H
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208[Hz]
X_Sweep = 7.53012048[kHz]
X_Sweep_Clipped = 6.02409639[kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 401.28219856[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scrunch = 32
Total_Scans = 32
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 19.8[dC]
X_90_Width = 9.25[us]
X_Acq_Time = 2.17579952[s]
X_Angle = 45[deg]
X_Atn = 0.8[dB]
X_Pulse = 4.625[us]
Tri_Mode = Off
Tri_Power = FALSE
Dante_Preset = 1[s]
Initial_Wait = 7.17579952[s]
Repetition_Time

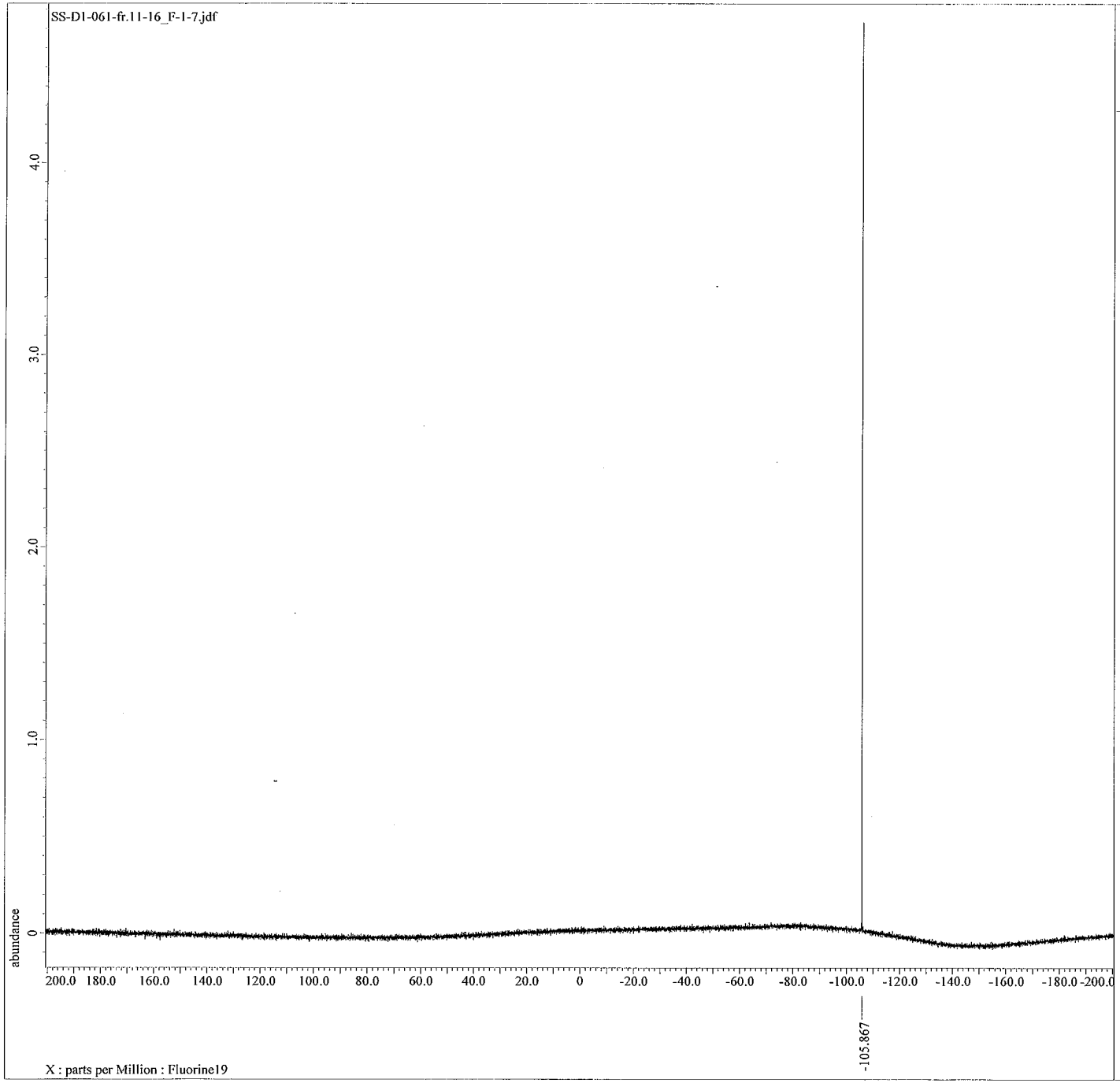



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = SS-D1-061-fr.11-16-C |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 9-MAY-2013 17:10:08 |
| Revision_Time | = 9-MAY-2013 19:04:21 |
| Current_Time | = 9-MAY-2013 19:04:41 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.5[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |

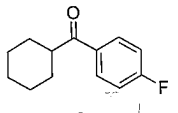



**3m**

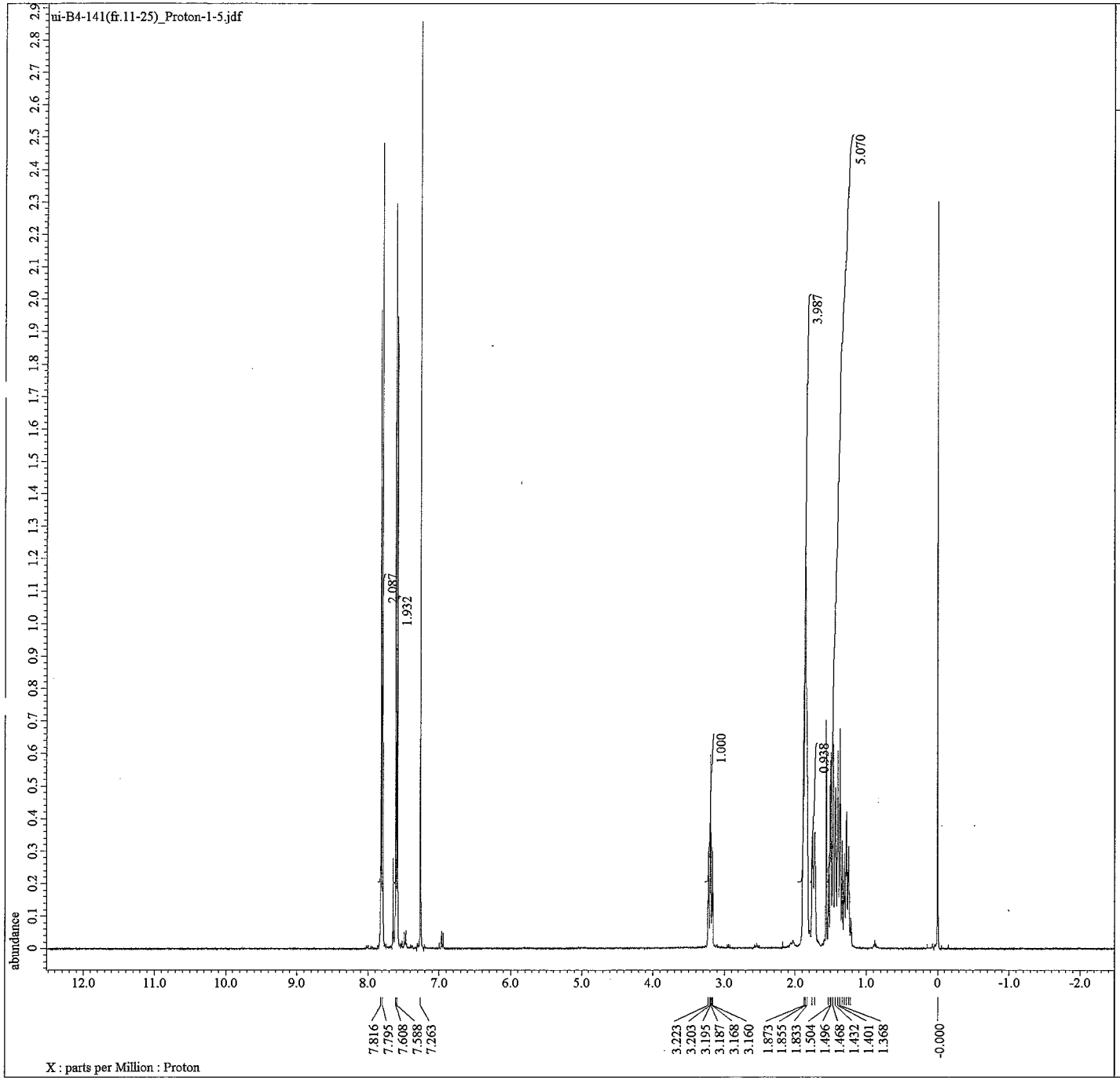



JEOL RESONANCE

| | |
|---|---|
| Filename | = C:\Users\delta\Documents\J |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = SS-D1-061-fr.11-16 |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 9-MAY-2013 17:37:31 |
| Revision_Time | = 10-MAY-2013 10:43:49 |
| Current_Time | = 10-MAY-2013 10:43:59 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Fluorine19 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 86.50752[ms] |
| X_Domain | = 19F |
| X_Freq | = 377.58246406[MHz] |
| X_Offset | = 0[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 11.55968868[Hz] |
| X_Sweep | = 189.39393939[kHz] |
| X_Sweep_Clipped | = 151.51515152[kHz] |
| Irr_Domain | = Fluorine19 |
| Irr_Freq | = 377.58246406[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Fluorine19 |
| Tri_Freq | = 377.58246406[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 16 |
| Total_Scans | = 16 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 48 |
| Temp_Get | = 20.3[dC] |
| X_90_Width | = 10.75[us] |
| X_Acq_Time | = 86.50752[ms] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 5.375[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 5.08650752[s] |

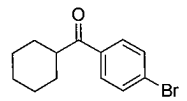



3m

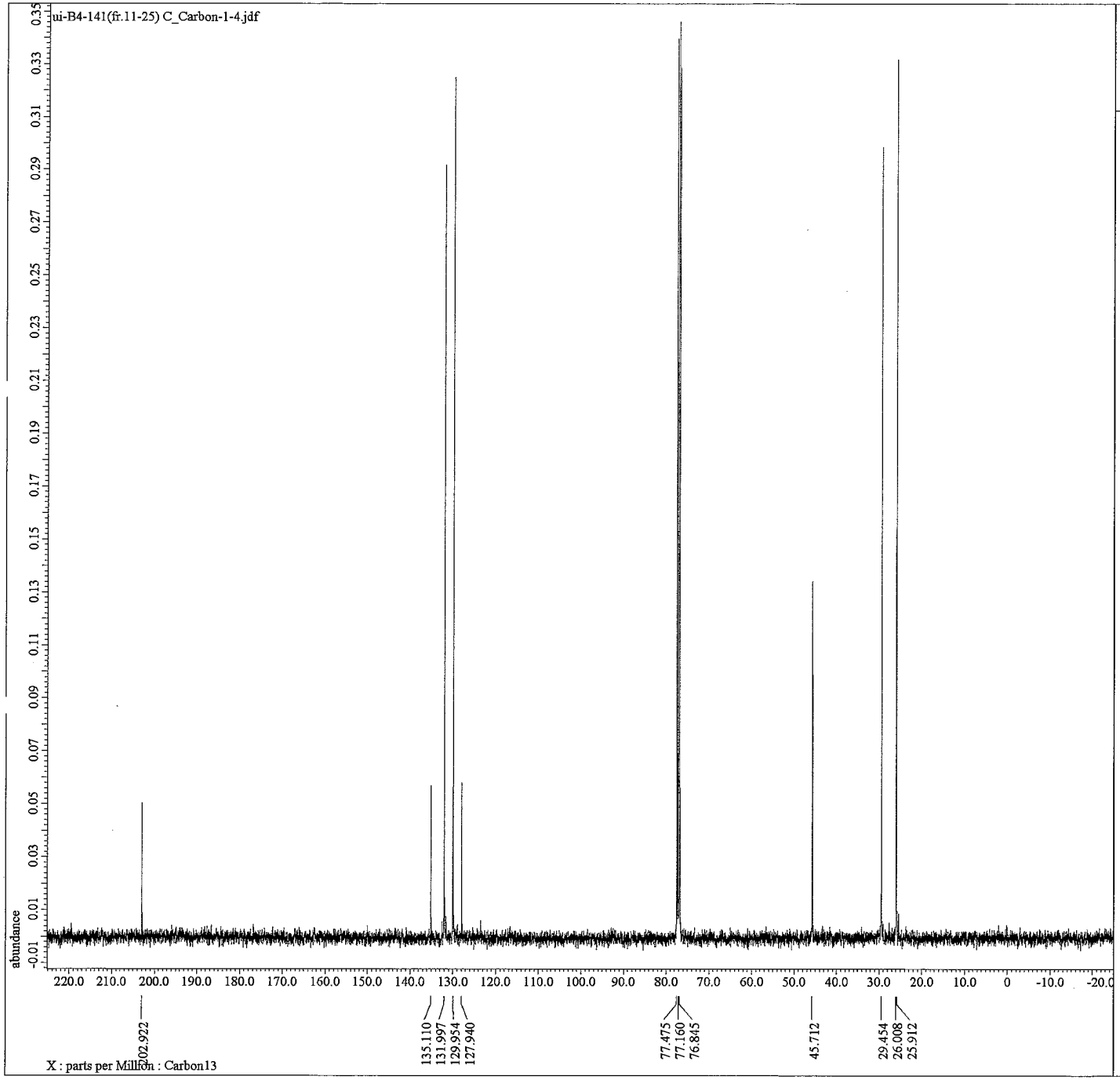



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-B4-141(fr.11-25) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 22-FEB-2013 17:07:55 |
| Revision_Time | = 14-MAR-2013 13:18:27 |
| Current_Time | = 14-MAR-2013 13:18:36 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.1757952[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 48 |
| Temp_Get | = 20.4[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.1757952[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.1757952[s] |

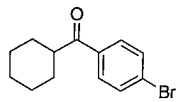



3n

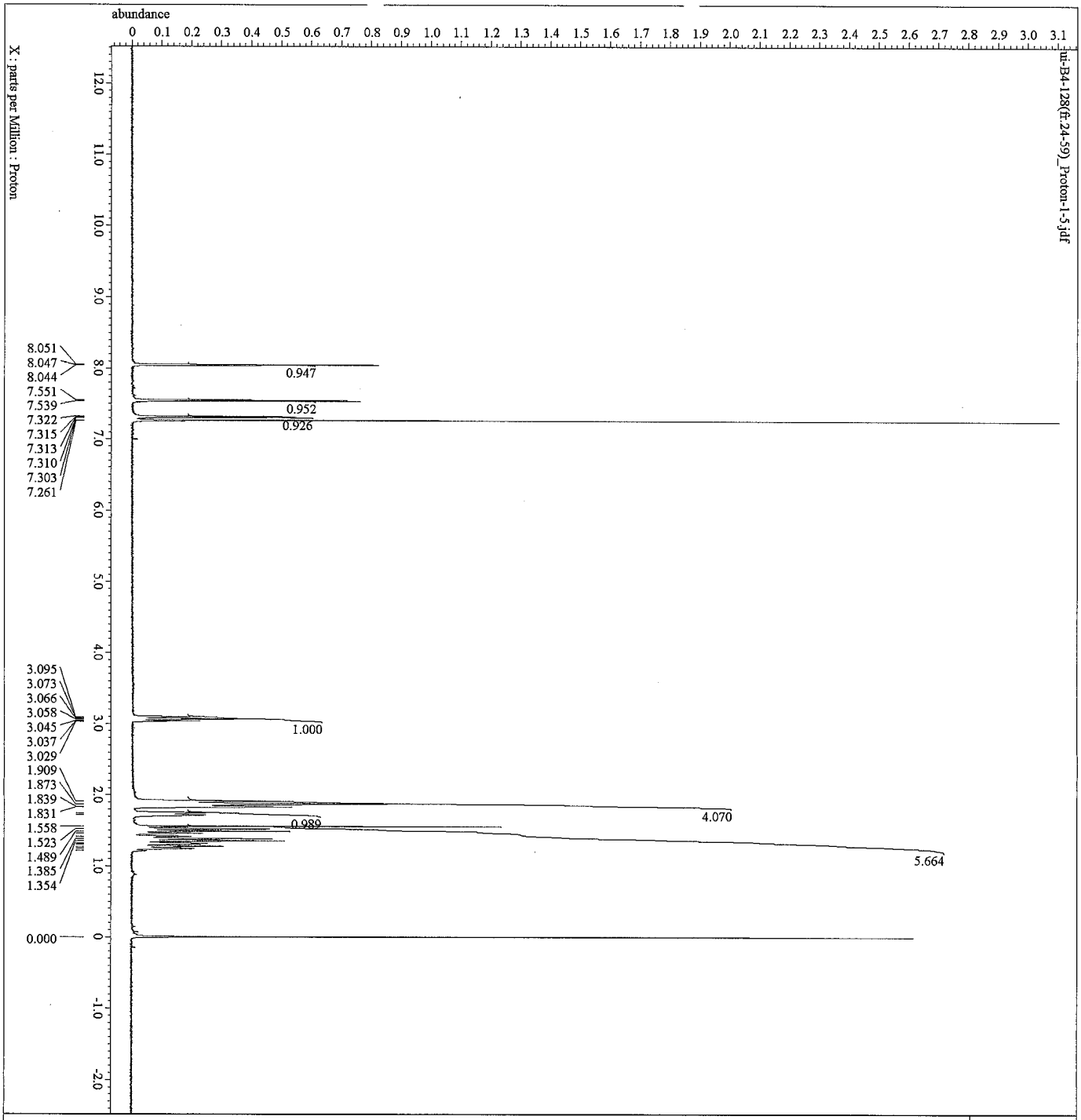



JEOL RESONANCE

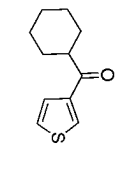
| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jkp |
| Sample_Id | = ui-B4-141(fr.11-25) C |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 22-FEB-2013 17:22:28 |
| Revision_Time | = 14-MAR-2013 13:19:08 |
| Current_Time | = 14-MAR-2013 13:19:21 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.3[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |



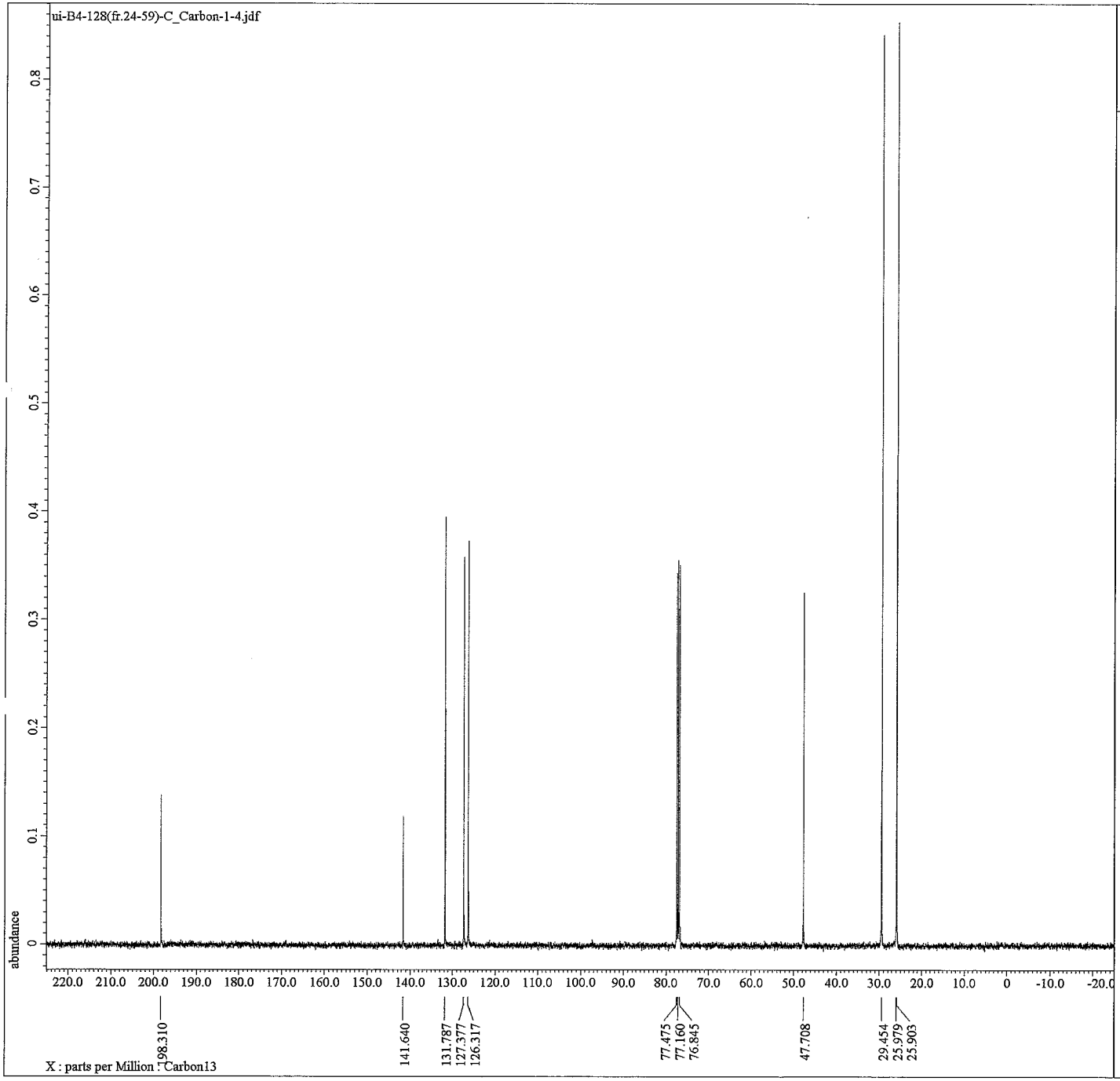

3n




```
Filename                = \\zeze\delta\Documents\VEO
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = ui-B4-128(ff.24-59)
Solvent                 = CHLOROFORM-D
Creation_Time           = 13-FEB-2013 18:22:26
Revision_Time           = 14-MAR-2013 13:30:27
Current_Time            = 14-MAR-2013 13:30:42

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.424996E1[T] (400[MHz])
X_Acq_Duration          = 2.17579520[s]
X_Domain                = 1H
X_Freq                  = 401.28219856[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45960208[Hz]
X_Sweep                 = 7.53012048[kHz]
X_Sweep_Clipped         = 6.02409639[kHz]
Irr_Domain              = Proton
Irr_Freq                = 401.28219856[MHz]
Irr_Offset              = 5[ppm]
Irr_Domain              = Proton
Tri_Freq                = 401.28219856[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 50
Temp_Get                = 20.3[dC]
X_90_Width              = 9.25[us]
X_Acq_Time              = 2.17579520[s]
X_Angle                 = 45[deg]
X_Atn                   = 0.8[dB]
X_Pulse                 = 4.625[us]
Irr_Mode                = off
Tri_Mode                = off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.17579520[s]
```

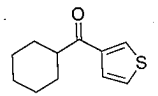


3o

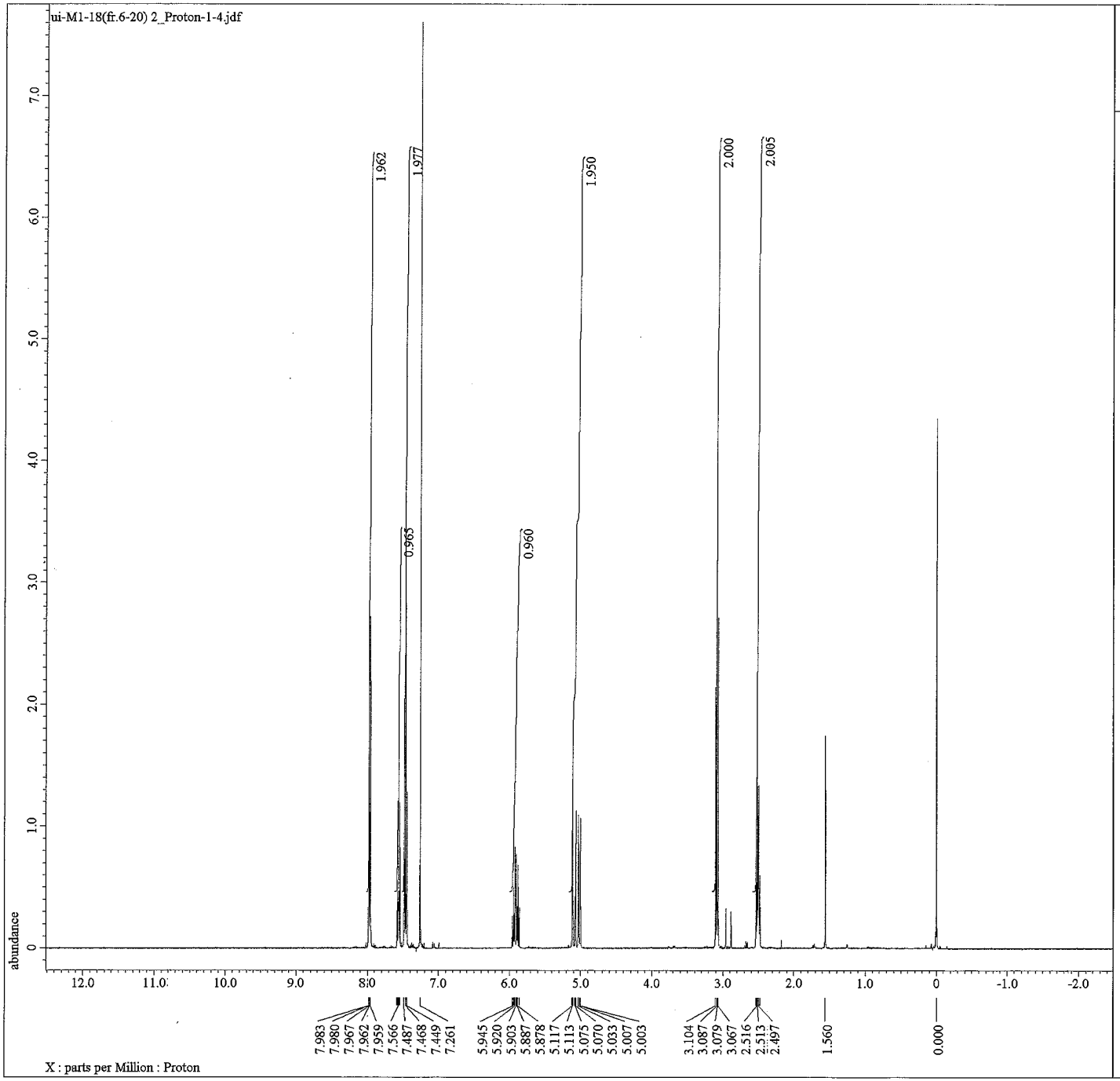



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = ui-B4-128(fr.24-59)-C |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 13-FEB-2013 18:28:18 |
| Revision_Time | = 14-MAR-2013 13:31:40 |
| Current_Time | = 14-MAR-2013 13:31:50 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.5[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |

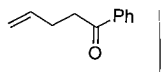



3o

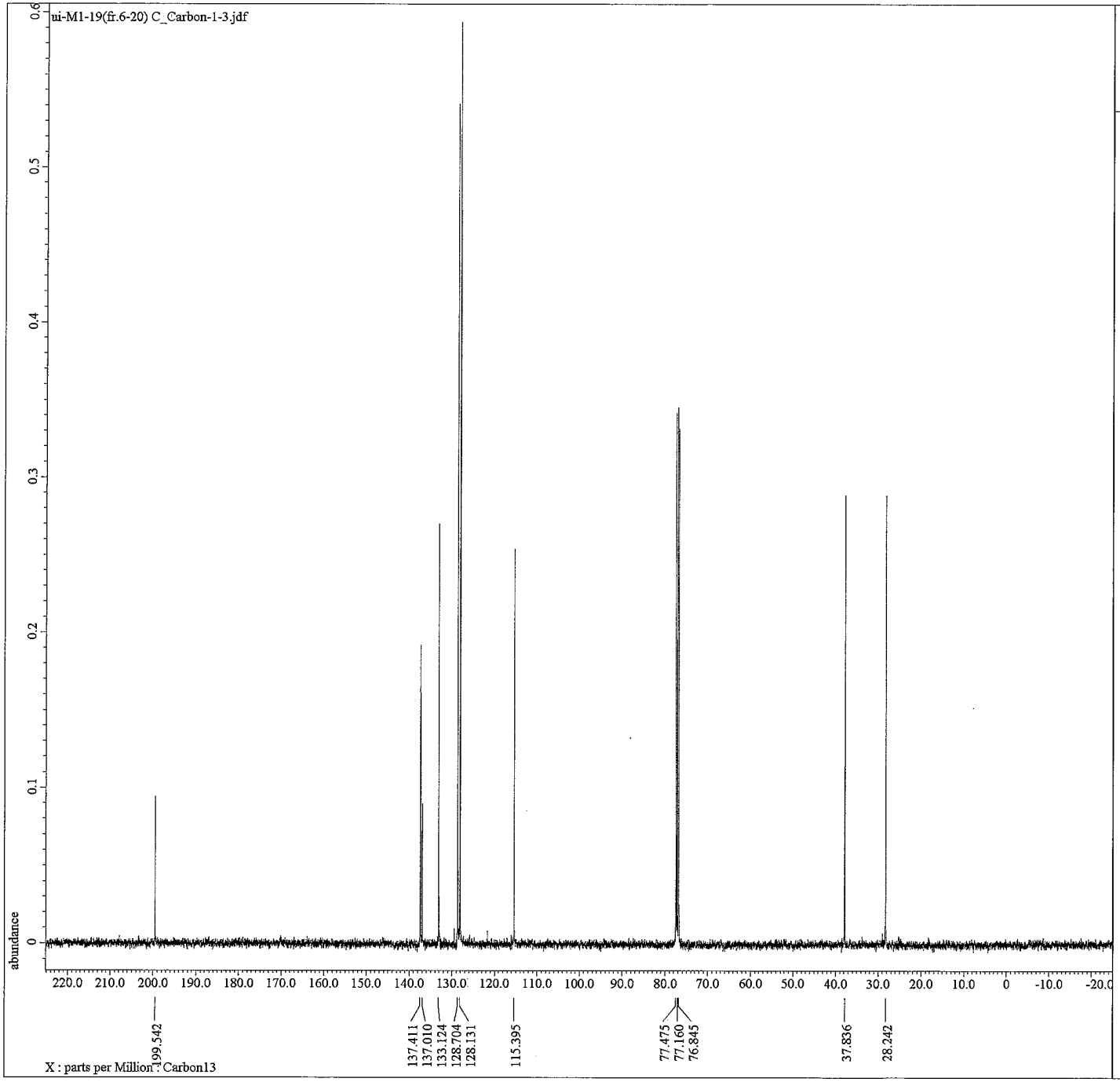



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-M1-18(fr.6-20) 2 |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 9-MAY-2013 18:26:09 |
| Revision_Time | = 9-MAY-2013 19:21:27 |
| Current_Time | = 9-MAY-2013 19:21:39 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.1757952[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.6[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.1757952[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.1757952[s] |

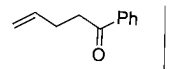



**3p**

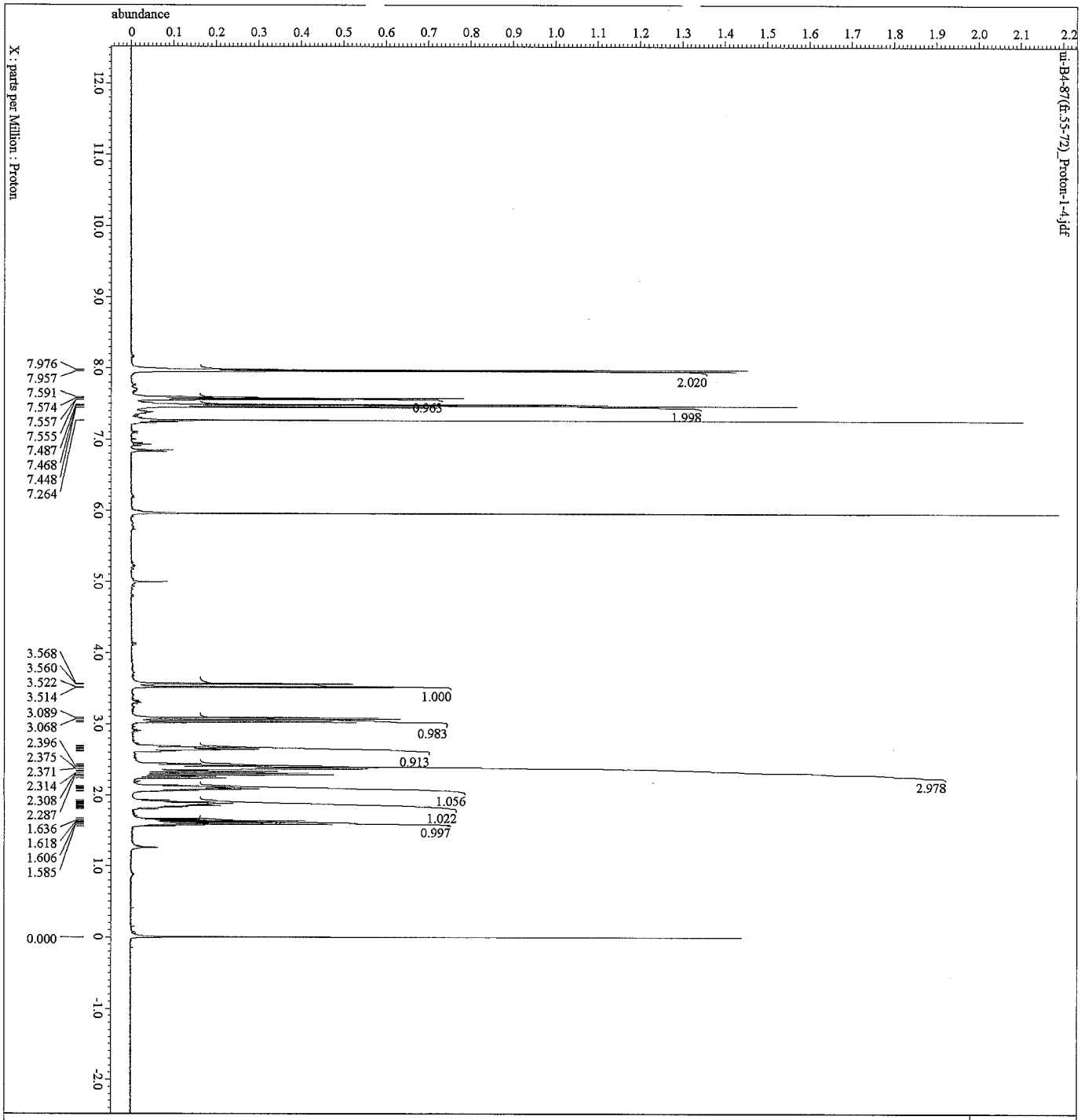



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = ui-M1-19(fr.6-20) C |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 9-MAY-2013 17:44:32 |
| Revision_Time | = 9-MAY-2013 19:19:26 |
| Current_Time | = 9-MAY-2013 19:19:45 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 256 |
| Total_Scans | = 256 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.8[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |

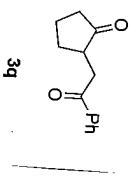



**3p**

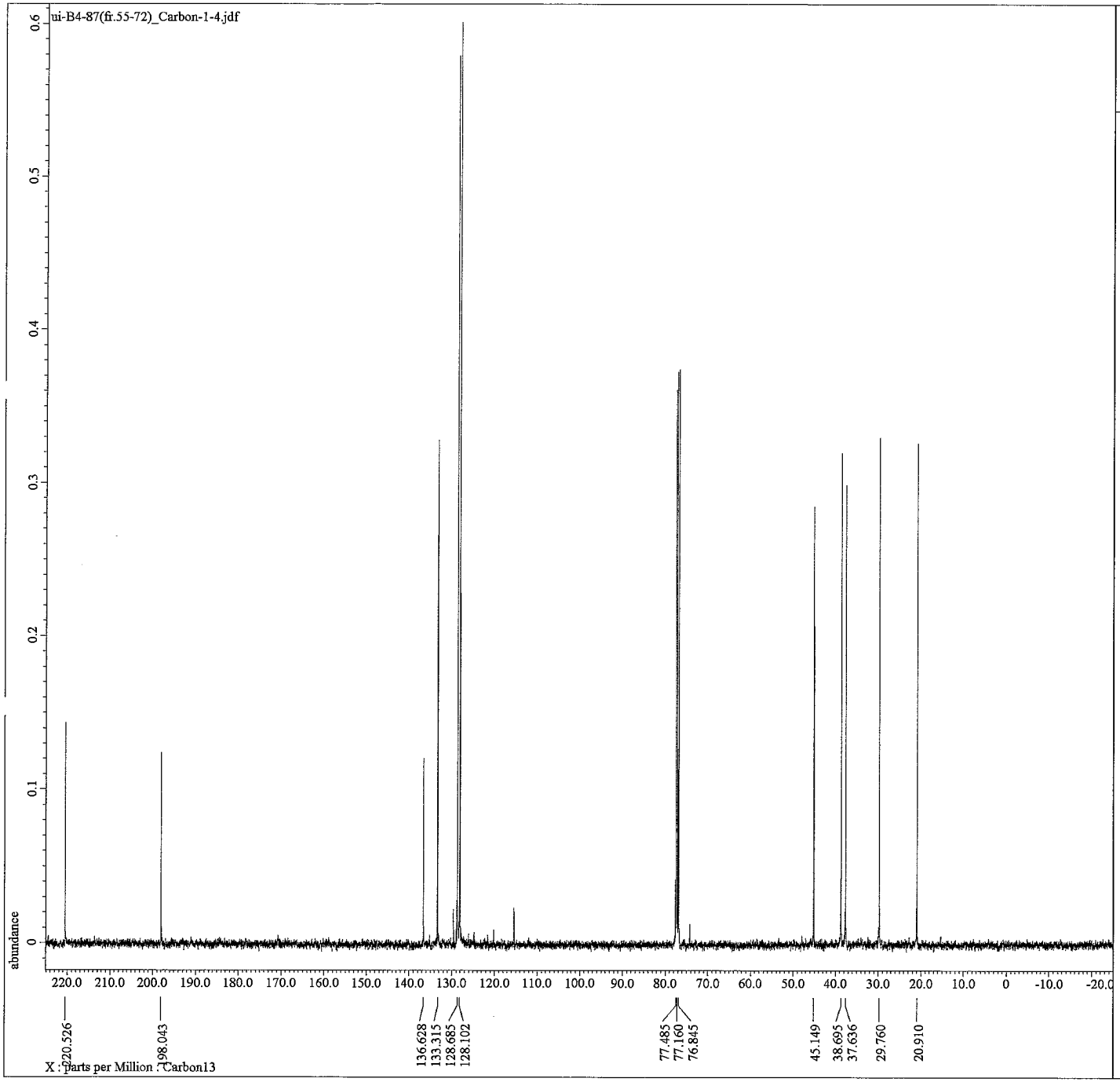



JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\NEO |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = ui-B4-87(ft.55-72) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 8-DEC-2012 18:11:48 |
| Revision_Time | = 14-MAR-2013 13:53:33 |
| Current_Time | = 14-MAR-2013 13:53:37 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 2.17579521[s] |
| X_Domain | = 1H |
| X_Freq | = 401.28219856[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45960208[Hz] |
| X_Sweep | = 7.53012048[kHz] |
| X_Sweep_Clipped | = 6.02409639[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 401.28219856[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 16 |
| Total_Scans | = 16 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 46 |
| Temp_Get | = 20.2[dC] |
| X_90_Width | = 9.25[us] |
| X_Acq_Time | = 2.17579521[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.8[dB] |
| X_Pulse | = 4.625[us] |
| Irr_Mode | = off |
| Tri_Mode | = off |
| Dante_Presat | = FALSE |
| Initial_Wait | = 1[s] |
| Repetition_Time | = 7.17579521[s] |

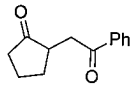



3q

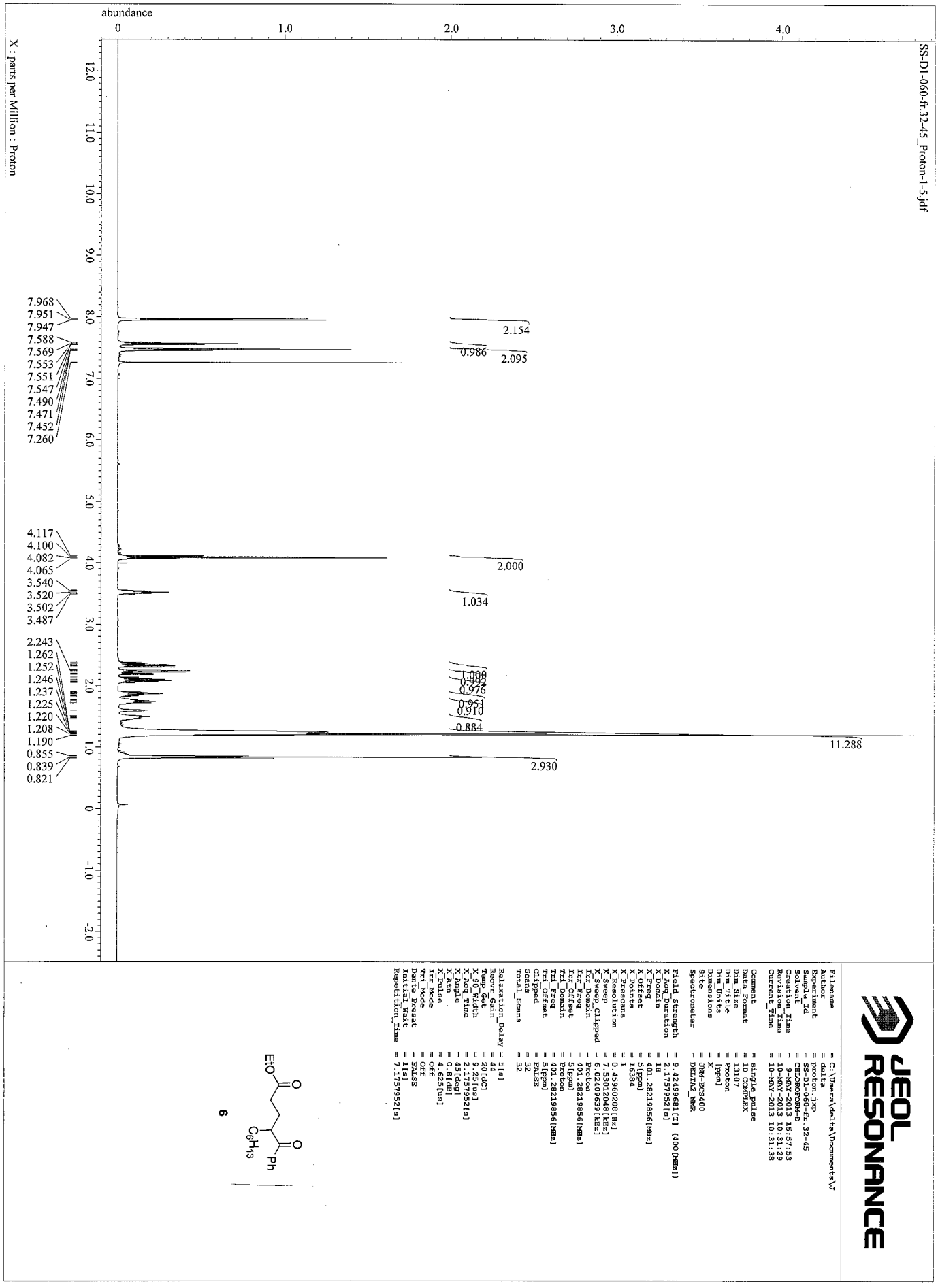


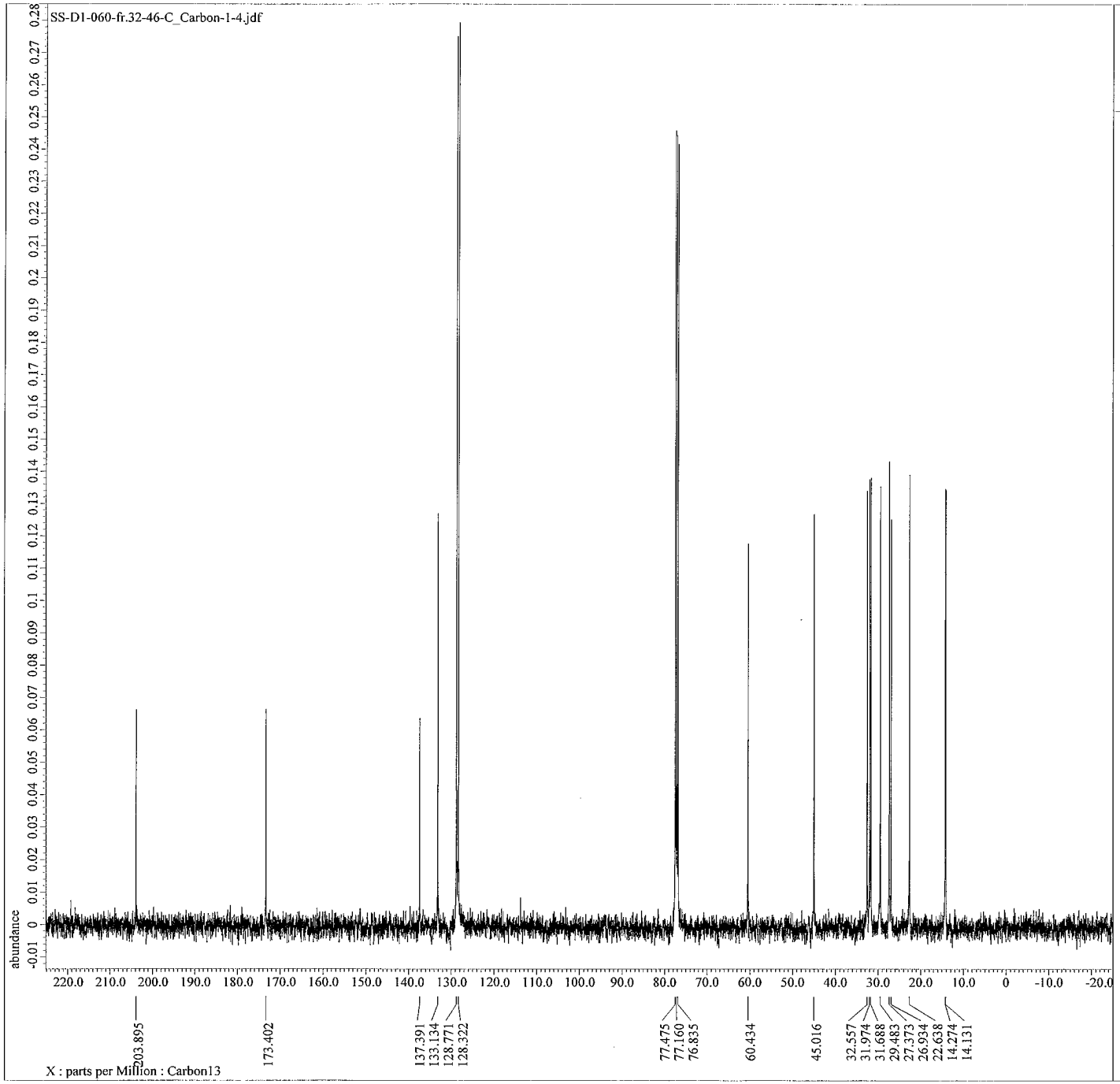

JEOL RESONANCE

| | |
|---|---|
| Filename | = \Users\delta\Documents\JEO |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = ui-B4-87(fr.55-72) |
| Solvent | = CHLOROFORM-D |
| Creation_Time | = 8-DEC-2012 21:37:34 |
| Revision_Time | = 14-MAR-2013 13:55:05 |
| Current_Time | = 14-MAR-2013 13:55:14 |
| Comment | = single pulse decoupled gat |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECS400 |
| Spectrometer | = DELTA2_NMR |
| Field_Strength | = 9.42499681[T] (400[MHz]) |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.90247863[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 401.28219856[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 254 |
| Total_Scans | = 254 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.5[dC] |
| X_90_Width | = 8.75[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 5.2[dB] |
| X_Pulse | = 2.91666667[us] |
| Irr_Atn_Dec | = 22.691[dB] |
| Irr_Atn_Noe | = 22.691[dB] |
| Irr_Noise | = WALTZ |
| Irr_Pwidth | = 0.115[ms] |
| Decoupling | = TRUE |
| Initial_Wait | = 1[s] |
| Noe | = TRUE |
| Noe_Time | = 2[s] |
| Repetition_Time | = 3.03809024[s] |



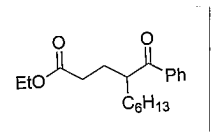

**3q**


abundance
X : parts per Million : Proton
SS-D1-060-fr.32-45_Proton-1-5.jdf
7.968
7.951
7.947
7.588
7.569
7.553
7.551
7.547
7.490
7.471
7.452
7.260
4.117
4.100
4.082
4.065
3.540
3.520
3.502
3.487
2.243
1.262
1.252
1.246
1.237
1.225
1.220
1.208
1.190
0.855
0.839
0.821
2.154
0.986
2.095
2.000
1.034
0.884
11.288
2.930
JEOL RESONANCE
Filename = C:\Users\delta\Documents\7
Author = delta
Experiment = proton.jxp
Sample_id = SS-D1-060-fr.32-45
Solvent = CHLOROFORM-D
Creation_Time = 9-MAY-2013 15:57:53
Revision_Time = 10-MAY-2013 10:31:29
Current_Time = 10-MAY-2013 10:31:38
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681[T] (400[MHz])
X_Acq_Duration = 2.17579552[s]
X_Domain = 1H
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960008[Hz]
X_Sweep = 7.53012048[kHz]
X_Sweep_clipped = 6.02409639[kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 401.28219856[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 20[dC]
X_90_Width = 9.25[us]
X_Acq_time = 2.17579552[s]
X_Angle = 45[deg]
X_Atn = 0.8[dB]
X_Pulse = 4.625[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_time = 7.17579552[s]
EtO
O
O
O
Ph
C6H13
6




JEOL RESONANCE

```
Filename          = \Users\delta\Documents\JEO
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = SS-D1-060-fr.32-46-C
Solvent           = CHLOROFORM-D
Creation_Time     = 10-MAY-2013 10:37:05
Revision_Time     = 10-MAY-2013 10:39:10
Current_Time      = 10-MAY-2013 10:39:27

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.42499681[T] (400[MHz])
X_Acq_Duration    = 1.03809024[s]
X_Domain          = 13C
X_Freq            = 100.90247863[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.96330739[Hz]
X_Sweep           = 31.56565657[kHz]
X_Sweep_Clipped   = 25.25252525[kHz]
Irr_Domain        = Proton
Irr_Freq          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 122
Total_Scans       = 122

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 20.9[dC]
X_90_Width        = 8.75[us]
X_Acq_Time        = 1.03809024[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 2.91666667[us]
Irr_Atn_Dec       = 22.69[dB]
Irr_Atn_Noe       = 22.69[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.03809024[s]
```




**6**