

Supporting Information

Versatile and sustainable alcoholysis of amides by reusable CeO₂ catalyst

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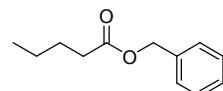
615-8520, Japan

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NMR and GC/MS analysis

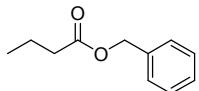
¹H and ¹³C NMR spectra for esters of Table-2 and Table-3 were assigned and reproduced to the corresponding literature. ¹H and ¹³C NMR spectra were recorded using at ambient temperature on JEOL-ECX 600 operating at 600.17 and 150.92 MHz, respectively with tetramethylsilane as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. All chemical shifts are reported relative to tetramethylsilane and d -solvent ($CDCl_3$) peaks respectively. Abbreviations used in the NMR experiments: s, singlet d, doublet; t, triplet; q, quartet; m, multiplet. GC-MS spectra was taken by SHIMADZU QP2010.

Pentanoic acid benzyl ester:¹



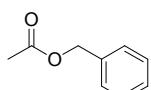
¹H NMR (600.17 MHz, $CDCl_3$, TMS): δ 7.37-7.33 (m, 4H), 7.32-7.29 (m, 1H), 5.10 (s, 2H), 2.35 (t, $J = 7.56$ Hz, 2H), 1.65-1.60 (m, 2H), 1.36-1.31 (m, 2H), 0.90 (t, $J = 7.56$ Hz, 3H); ¹³C NMR (150.92 MHz, $CDCl_3$) δ 173.67, 136.16, 128.54 (C \times 2), 128.15 (C \times 3), 66.05, 34.05, 27.01, 22.26, 13.71; GC-MS m/e 192.110.

Butyric acid benzyl ester:²



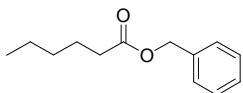
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.35-7.34 (m, 4H), 7.32-7.30 (m, 1H), 5.11 (s, 2H), 2.33 (t, *J* = 7.56 Hz, 2H), 1.69-1.65 (m, 2H), 0.94 (t, *J* = 7.56 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 173.51, 136.15, 128.54(C×2), 128.16 (C×3), 66.04, 36.19, 18.44, 13.67; GC-MS m/e 178.105.

Acetic acid benzyl ester:³



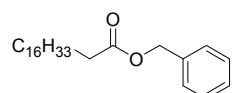
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.35-7.34 (m, 4 H), 7.32-7.30 (m, 1H), 5.10 (s, 2H), 2.08 (s, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 170.86, 135.95, 128.56 (C×2), 128.26 (C×3), 66.29, 20.99; GC-MS m/e 150.055.

Hexanoic acid benzyl ester:⁴



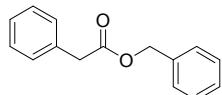
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.38-7.35 (m, 4H), 7.34-7.31 (m, 1H), 5.12 (s, 2H), 2.35 (t, *J* = 7.56 Hz, 2H), 1.68-1.64 (m, 2H), 1.33-1.26 (m, 4H), 0.89 (t, *J* = 7.56 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 173.65, 136.17, 128.53 (C×2), 128.16(C×3), 66.04, 34.28, 31.30, 24.64, 22.32, 13.90; GC-MS m/e 206.135.

Octadecanoic acid benzyl ester:⁵



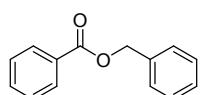
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.36-7.34 (m, 4H), 7.32-7.31 (m, 1H), 2.34 (t, *J* = 7.56 Hz, 2H), 1.64-1.62 (m, 2H), 1.28-1.24 (m, 28H), 0.88 (t, *J* = 6.60 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 173.67, 136.10, 128.50 (C×2), 128.12 128.32 (C×2), 66.01, 34.30, 31.91, 29.68(C×4), 29.65(C×2), 29.56, 29.43, 29.34, 29.23, 29.10, 24.93, 22.67, 14.10; GC-MS m/e 374.320.

Phenyl-acetic acid benzyl ester:⁶



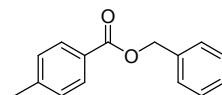
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.35-7.25 (m, 10H), 5.12 (s, 2H), 3.66 (s, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 171.36, 135.83, 133.87, 129.27 (C×2), 128.56 (C×2), 128.51 (C×2), 128.19, 128.10 (C×2), 127.10, 66.58, 41.31 ; GC-MS m/e 226.105.

Benzoic acid benzyl ester:⁷



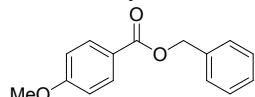
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.08 (d, *J*= 8.88 Hz, 2H), 7.55-7.53 (m, 1H), 7.45-7.41 (m, 4H), 7.39-7.37 (m, 2H), 7.35-7.33 (m, 1H), 5.35 (s, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.40, 136.05, 133.01, 130.13, 129.69 (C×2), 128.58 (C×2), 128.36 (C×2), 128.23, 128.15 (C×2), 66.66; GC-MS m/e 212.090.

4-Methyl-benzoic acid benzyl ester:⁸



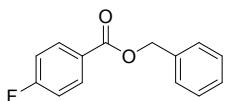
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.96 (d, *J*= 8.28 Hz, 2H), 7.43 (d, *J*= 7.56 Hz, 2H), 7.36-7.34 (m, 2H), 7.33-7.29 (m, 1H), 7.20 (d, *J*= 6.84 Hz, 2H), 5.34 (s, 2H), 2.39 (s, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.50, 143.71, 136.21, 129.74 (C×2), 129.09 (C×2), 129.01 (C×2), 128.57 (C×2), 128.17 (C×2), 128.12, 127.40, 66.50, 21.66; GC-MS m/e 226.105.

4-Methoxy-benzoic acid benzyl ester:⁹



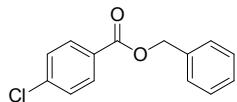
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.03 (d, *J*= 8.88 Hz, 2H), 7.43 (d, *J*= 7.56 Hz, 2H), 7.38-7.36 (m, 2H), 7.33-7.32 (m, 1H), 6.90 (d, *J*= 8.88 Hz, 2H), 5.33 (s, 2H), 3.83 (s, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.16, 163.42, 136.30, 131.73 (C×3), 128.55 (C×2), 128.12 (C×2), 128.08 (C×2), 122.53, 113.61 (C×2), 66.37, 55.39 ; GC-MS m/e 242.095.

4-Fluoro-benzoic acid benzyl ester:¹⁰



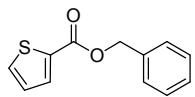
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.09-8.07 (m, 2H), 7.44-7.42(m, 2H), 7.39-7.37 (m, 2H), 7.35-7.32(m, 1H), 7.10-7.07 (m, 2H), 5.34 (s, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 165.82 (d, *J*= 252.88 Hz, 4-F-C), 165.45, 135.91, 132.26 (d, *J*= 10.11 Hz, *meta* to 4-F, C×2), 128.63 (C×2), 128.34, 128.23 (C×2), 126.37, 115.53 (d, *J*= 21.68 Hz, *ortho* to 4-F, C×2), 66.84; GC-MS m/e 230.070.

4-Chloro-benzoic acid benzyl ester:¹¹



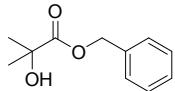
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.99 (d, *J*= 8.88 Hz, 2H), 7.43 (d, *J*= 7.56 Hz, 2H), 7.39-7.37 (m, 4H), 7.35-7.33 (m, 1H), 5.34 (s, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 165.53, 139.76, 136.36, 131.08 (C×2), 128.71 (C×2), 128.63 (C×2), 128.57, 128.35, 128.23 (C×2), 66.87; GC-MS m/e 246.045.

Thiophene-2-carboxylic acid benzyl ester:¹²



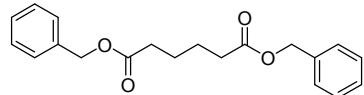
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.83-7.82 (m, 1H), 7.53 (dd, *J*= 4.80, 1.38 Hz, 1H), 7.43 (dd, *J*= 4.80, 1.38 Hz, 2H), 7.37 (t, *J*= 6.90 Hz, 2H), 7.34 (t, *J*= 7.56 Hz, 1H), 7.08 (t, *J*= 4.80 Hz, 1H), 5.33 (s, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 162.04, 135.82, 133.63, 133.50, 132.54, 128.57 (C×2), 128.27, 128.14 (C×2), 127.75, 66.70; GC-MS m/e 218.045.

2-Hydroxy-2-methyl-propionic acid benzyl ester:¹³



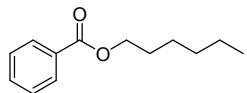
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.37-7.34 (m, 5H), 5.19 (s, 2H), 3.16 (br s, 1H), 1.44 (s, 6H); ¹³C NMR (150.92 MHz, CDCl₃) δ 177.26, 135.41, 128.64 (C×2), 128.45 (C×2), 128.00, 72.09, 67.36, 27.16; GC-MS m/e 194.100.

Hexanedioic acid dibenzyl ester:¹⁴



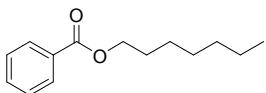
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 7.35-7.32 (m, 10H), 5.10 (s, 4H), 2.37-2.35 (m, 4H), 1.68-1.67 (m, 4H); ¹³C NMR (150.92 MHz, CDCl₃) δ 173.09 (C×2) , 135.99 (C×2), 128.56 (C×6), 128.20 (C×4), 66.19 (C×2), 33.86 (C×2), 24.33 (C×2); GC-MS m/e 326.150.

Benzoic acid hexyl ester:¹⁵



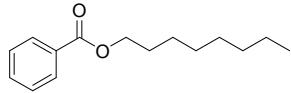
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.04 (d, *J*= 8.22 Hz, 2H), 7.55 (t, *J*= 7.38 Hz, 1H), 7.43 (t, *J*= 7.56 Hz, 2H), 4.31 (t, *J*= 6.90 Hz, 2H), 1.77-1.75 (m, 2H), 1.45-1.43 (m, 2H), 1.35-1.33 (m, 4H), 0.90 (t, *J*= 6.90 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.70, 132.78, 130.55, 129.54 (C×2), 128.31 (C×2), 65.14, 31.48, 28.71, 25.73, 22.57, 14.02; GC-MS m/e 206.135.

Benzoic acid heptyl ester :¹⁶



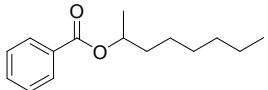
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.04 (d, *J*= 8.22 Hz, 2H), 7.54 (t, *J*= 7.56 Hz, 1H), 7.43 (t, *J*= 7.56 Hz, 2H), 4.31 (t, *J*= 6.18 Hz, 2H), 1.79-1.74 (m, 2H), 1.45-1.41 (m, 2H), 1.36-1.25 (m, 6H), 0.88 (t, *J*= 6.90 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.69, 132.78, 130.57, 129.54 (C×2), 128.32 (C×2), 65.14, 31.76, 28.99, 28.75, 26.03, 22.61, 14.08; GC-MS m/e 220.150.

Benzoic acid octyl ester:¹⁷



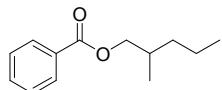
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.04 (d, *J*= 8.28 Hz, 2H), 7.54 (t, *J*= 7.56 Hz, 1H), 7.43 (t, *J*= 7.56 Hz, 2H), 4.31 (t, *J*= 6.87 Hz, 2H), 1.77-1.74 (m, 2H), 1.45-1.42 (m, 2H), 1.35-1.27 (m, 8H), 0.89 (t, *J*= 7.56 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.69, 132.78, 130.57, 129.54 (C×2), 128.32 (C×2), 65.15, 31.81, 29.28, 29.22, 28.75, 26.07, 22.66, 14.10; GC-MS m/e 234.165.

Benzoic acid 1-methyl-heptyl ester:¹⁸



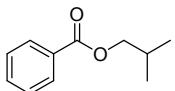
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.04 (d, *J*= 7.56 Hz, 2H), 7.54 (t, *J*= 6.90 Hz, 1H), 7.43 (t, *J*= 7.56 Hz, 2H), 5.16-5.14 (m, 1H), 1.74-1.70 (m, 1H), 1.62-1.58 (m, 1H), 1.39-1.26 (m, 11H), 0.87 (t, *J*= 6.90 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.23, 132.67, 130.94, 129.51 (C×2), 128.27 (C×2), 71.75, 36.08, 31.75, 29.18, 25.42, 22.60, 20.08, 14.07; GC-MS m/e 234.165.

Benzoic acid 2-methyl-pentyl ester:¹⁹



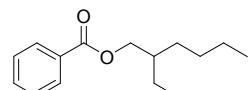
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.04 (d, *J*= 8.22 Hz, 2H), 7.55 (t, *J*= 6.90 Hz, 1H), 7.44 (t, *J*= 8.22 Hz, 2H), 4.22-4.19 (m, 1H), 4.12-4.09 (m, 1H), 1.97-1.93 (m, 1H), 1.46-1.42 (m, 2H), 1.36-1.33 (m, 1H), 1.25-1.22 (m, 1H), 1.02 (d, *J*= 6.84 Hz, 3H), 0.92 (t, *J*= 4.58 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.69, 132.80, 130.54, 129.53 (C×2), 128.34 (C×2), 69.87, 35.70, 32.46, 20.00, 17.00, 14.27; GC-MS m/e 206.135.

Benzoic acid isobutyl ester:²⁰



¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.05 (d, *J*= 7.52 Hz, 2H), 7.54 (t, *J*= 6.90 Hz, 1H), 7.42 (t, *J*= 7.56 Hz, 2H), 4.10 (d, *J*= 6.84 Hz, 2H), 2.09-2.07 (m, 1H), 1.01 (d, *J*= 6.18 Hz, 6H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.60, 132.81, 130.53, 129.54 (C×2), 128.33 (C×2), 70.99, 27.91, 19.20 (C×2); GC-MS m/e 178.100.

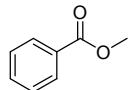
Benzoic acid 2-ethyl-hexyl ester:²⁰



¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.04 (d, *J*= 7.56 Hz, 2H), 7.55 (t, *J*= 6.90 Hz, 1H), 7.43 (t, *J*= 7.56 Hz, 2H), 4.24-4.23 (m, 2H), 1.73-1.71 (m, 1H), 1.48-1.43 (m, 2H), 1.40-1.39 (m, 2H), 1.34-1.32 (m, 4), 0.95 (t, *J*= 7.56 Hz, 3H), 0.90 (t, *J*= 6.90 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.76, 132.79, 130.59, 129.53 (C×2), 128.34 (C×2), 67.31, 38.95, 30.61, 29.01, 24.02,

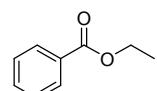
23.00, 14.06, 11.11; GC-MS m/e 234.165.

Benzoic acid methyl ester:²¹



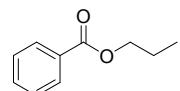
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.03 (d, *J*= 6.90 Hz, 2H), 7.56-7.53 (m, 1H), 7.44-7.41 (m, 2H), 3.91(s, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 167.11, 132.91, 130.15, 129.57 (C×2), 128.35 (C×2), 52.09; GC-MS m/e 136.055.

Benzoic acid ethyl ester:²²



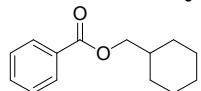
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.04 (d, *J*= 6.84 Hz, 2H), 7.55-7.53 (m, 1H), 7.44-7.42 (m, 2H), 4.28 (t, *J*= 7.23 Hz, 2H), 1.39 (t, *J*= 7.18 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.65, 132.81, 130.49, 129.53 (C×2), 128.30 (C×2), 60.95, 14.33; GC-MS m/e 150.070.

Benzoic acid propyl ester:²²



¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.05 (d, *J*= 7.84 Hz, 2H), 7.55-7.53 (m, 1H), 7.44-7.42 (m, 2H), 4.28 (t, *J*= 7.23 Hz, 2H), 1.80-1.77 (m, 2H), 1.03 (t, *J*= 6.90 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.69, 132.81, 130.53, 129.54 (C×2), 128.33 (C×2), 66.54, 22.12, 10.54; GC-MS m/e 212.095. GC-MS m/e 164.080.

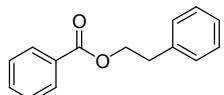
Benzoic acid cyclohexylmethyl ester:²³



¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.05 (d, *J*= 6.90 Hz, 2H), 7.54 (t, *J*= 7.56 Hz, 1H), 7.43 (t, *J*= 7.56 Hz, 2H), 4.13 (d, *J*= 6.18 Hz, 2H), 1.84-1.81 (m, 2H), 1.78-1.74 (m, 3H), 1.70-1.68 (m, 1H), 1.30-1.25 (m, 2H), 1.22-1.18 (m, 1H), 1.10-1.05 (m, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.66, 132.78, 130.57, 129.54 (C×2), 128.32 (C×2), 70.06, 37.29, 29.77 (C×2), 26.39, 25.73 (C×2);

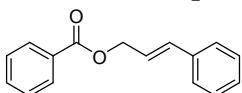
GC-MS m/e 218.135.

Benzoic acid phenethyl ester:²⁴



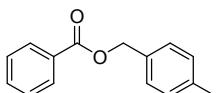
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.01 (d, *J*= 7.56 Hz, 2H), 7.52 (t, *J*= 7.56 Hz, 1H), 7.41 (t, *J*= 7.56 Hz, 2H), 7.32-7.27 (m, 4H), 7.24-7.21 (m, 1H), 4.52 (t, *J*= 6.90 Hz, 2H), 3.06 (t, *J*= 6.90 Hz, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.49, 137.90, 132.89, 130.28, 129.55 (C×2), 128.96 (C×2), 128.54 (C×2), 128.35 (C×2), 126.58, 65.46, 35.23; GC-MS m/e 226.100.

Benzoic acid 3-phenyl-allyl ester:²⁵



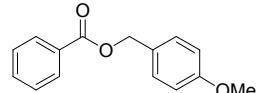
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.08 (t, *J*= 7.56 Hz, 2H), 7.55 (t, *J*= 7.56 Hz, 1H), 7.45-7.40 (m, 4H), 7.33-7.31 (m, 2H), 7.27-7.25 (m, 1H), 6.73 (d, *J*= 15.84 Hz, 1H), 6.43-6.39 (m, 1H), 4.98 (d, *J*= 6.84 Hz, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.39, 136.20, 134.26, 133.0, 132.14, 130.19, 129.66, 129.10, 128.61 (C×2), 128.37 (C×2), 128.09, 126.64, 123.24, 65.53; GC-MS m/e 238.100.

Benzoic acid 4-methyl-benzyl ester:²⁶



¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.05 (d, *J*= 7.56 Hz, 2H), 7.53 (t, *J*= 7.56 Hz, 1H), 7.41 (t, *J*= 7.56 Hz, 2H), 7.33 (d, *J*= 8.22 Hz, 2H), 7.18 (d, *J*= 7.56 Hz, 2H), 5.32 (s, 2H), 2.35 (s, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.46, 138.07, 133.04, 132.95, 130.22, 129.68 (C×2), 129.26 (C×2), 128.35 (C×2), 128.32 (C×2), 66.65, 21.20; GC-MS m/e 226.100.

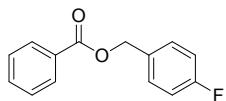
Benzoic acid 4-methoxy-benzyl ester:²⁷



¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.05 (d, *J*= 6.90 Hz, 2H), 7.51 (t, *J*= 7.56 Hz, 1H), 7.42-7.37 (m, 4H), 6.91 (d, *J*= 8.22 Hz, 2H), 5.29 (s, 2H), 3.79 (s, 3H); ¹³C NMR (150.92 MHz,

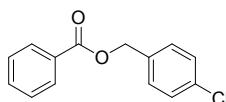
CDCl_3) δ 166.48, 159.64, 132.92, 130.25, 130.06 ($\text{C} \times 2$), 129.66 ($\text{C} \times 2$), 128.32 ($\text{C} \times 2$), 128.15, 113.96 ($\text{C} \times 2$), 66.52, 55.25; GC-MS m/e 226.100.

Benzoic acid 4-fluoro-benzyl ester:²⁸



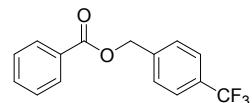
^1H NMR (600.17 MHz, CDCl_3 , TMS): δ 8.06 (d, $J = 8.28$ Hz, 2H), 7.55 (t, $J = 7.56$ Hz, 1H), 7.44-7.42 (m, 4H), 7.06 (t, $J = 8.28$ Hz, 2H), 5.32 (s, 2H); ^{13}C NMR (150.92 MHz, CDCl_3) δ 166.37, 162.66 (d, $J = 247.08$ Hz, 4-F-C), 133.11, 131.90, 130.20 (d, $J = 8.68$ Hz, *meta* to 4-F, $\text{C} \times 2$), 130.0, 129.68 ($\text{C} \times 2$), 128.40 ($\text{C} \times 2$), 115.52 (d, $J = 20.24$ Hz, *ortho* to 4-F, $\text{C} \times 2$), 65.98; GC-MS m/e 230.070.

Benzoic acid 4-chloro-benzyl ester:²⁹



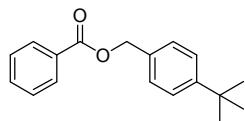
^1H NMR (600.17 MHz, CDCl_3 , TMS): δ 8.06 (d, $J = 8.28$ Hz, 2H), 7.55 (t, $J = 7.56$ Hz, 1H), 7.43 (t, $J = 7.56$ Hz, 2H), 7.38-7.34 (m, 4H), 5.31 (s, 2H); ^{13}C NMR (150.92 MHz, CDCl_3) δ 166.29, 134.55, 134.12, 133.16, 129.89, 129.67 ($\text{C} \times 2$), 129.56 ($\text{C} \times 2$), 128.78 ($\text{C} \times 2$), 128.42 ($\text{C} \times 2$), 65.85; GC-MS m/e 246.045.

Benzoic acid 4-trifluoromethyl-benzyl ester:³⁰



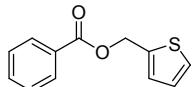
^1H NMR (600.17 MHz, CDCl_3 , TMS): δ 8.07 (d, $J = 6.84$ Hz, 2H), 7.64 (d, $J = 7.56$ Hz, 2H), 7.57-7.55 (m, 3H), 7.44 (t, $J = 7.56$ Hz, 2H), 5.41 (s, 2H); ^{13}C NMR (150.92 MHz, CDCl_3) δ 166.26, 140.11, 133.33, 130.77 (q, $J = 33.23$ Hz), 129.75 ($\text{C} \times 2$), 128.52 ($\text{C} \times 2$), 128.14 ($\text{C} \times 2$), 125.63 (d, $J = 4.33$ Hz, $\text{C} \times 2$), 124.97, 123.16 (d, $J = 271.67$ Hz, $\text{C} \times 2$), 66.23; GC-MS m/e 280.075.

Benzoic acid 4-*tert*-butyl-benzyl ester³¹



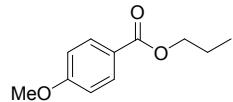
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.07 (d, *J* = 6.18 Hz, 2H), 7.54 (t, *J* = 7.56 Hz, 1H), 7.43-7.39 (m, 6H), 5.34 (s, 2H), 1.32 (s, 9H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.47, 151.27, 133.03, 132.95, 132.13, 129.68 (C×2), 128.32 (C×2), 128.10 (C×2), 125.50 (C×2), 65.54, 34.59, 31.05 (C×3); GC-MS m/e 268.145.

Benzoic acid thiophen-2-yl methyl ester:³²



¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.05 (d, *J* = 6.90 Hz, 2H), 7.53 (t, *J* = 7.56 Hz, 1H), 7.40 (t, *J* = 7.56 Hz, 2H), 7.31 (d, *J* = 4.8 Hz, 1H), 7.16 (d, *J* = 3.4 Hz, 1H), 6.99 (t, *J* = 3.4 Hz, 1H), 5.50 (s, 2H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.22, 137.99, 133.08, 129.90, 129.72 (C×2), 128.35 (C×2), 128.18, 126.84, 126.82, 61.01; GC-MS m/e 218.045.

4-Methoxy-benzoic acid propyl ester:³³

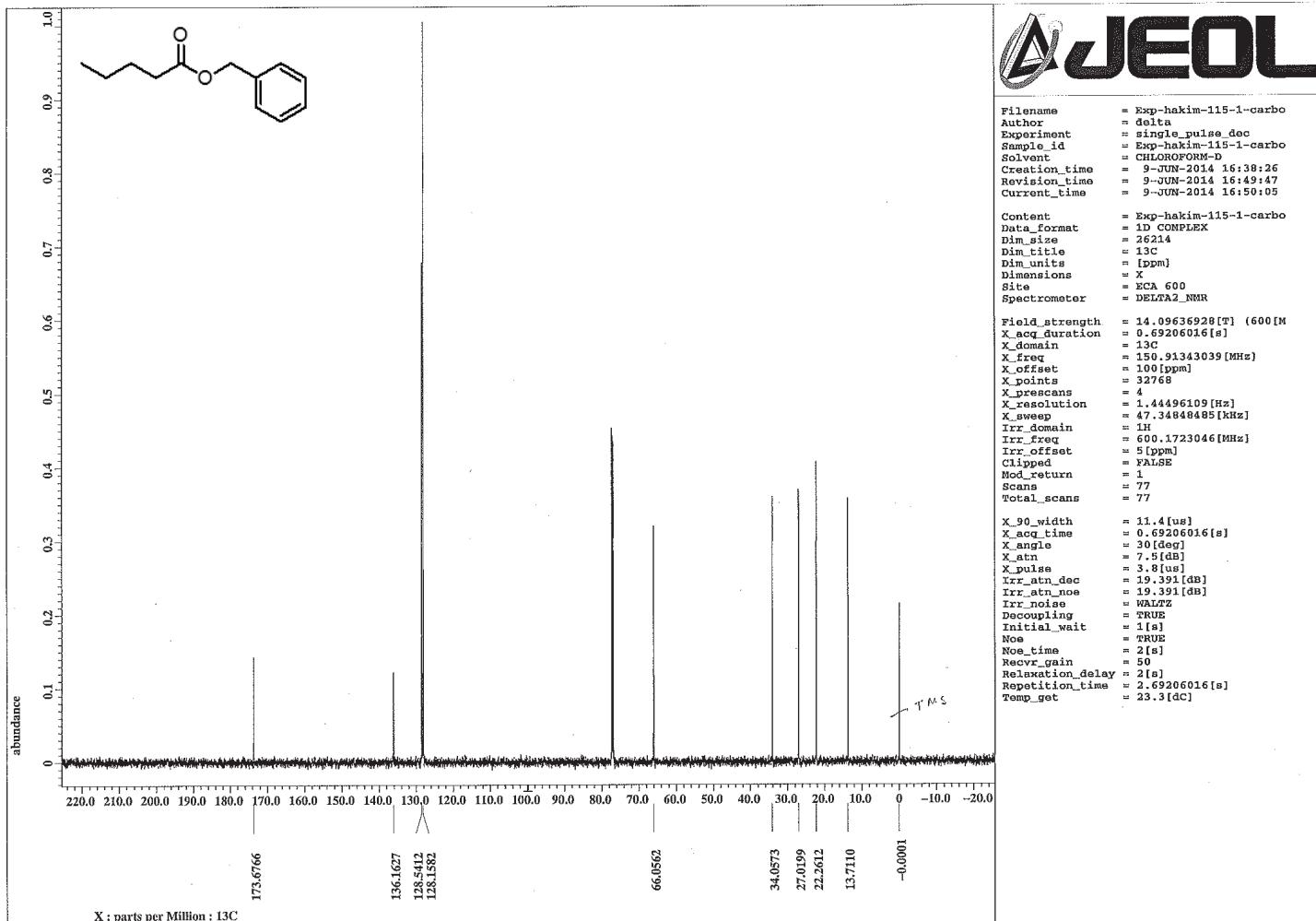
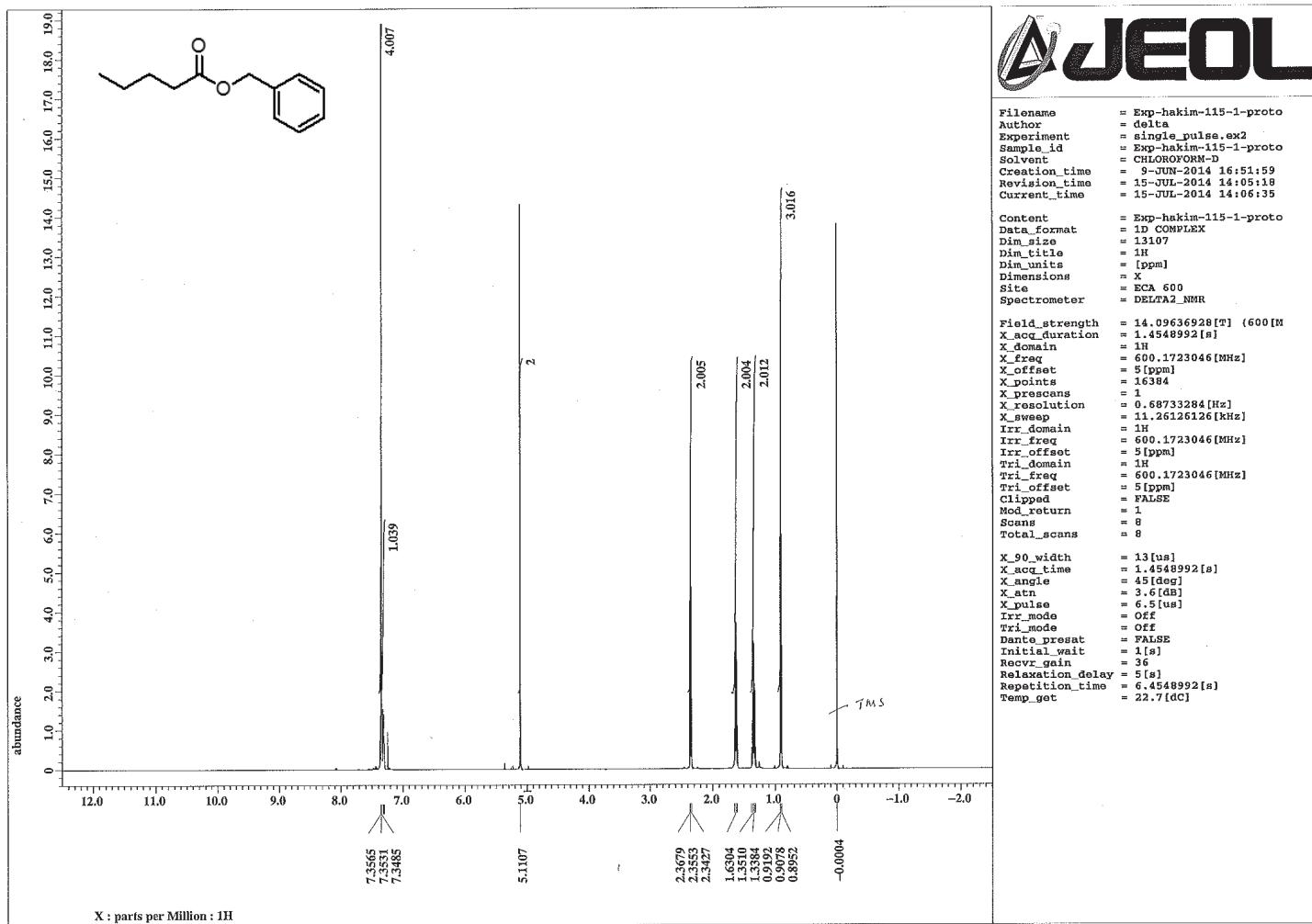


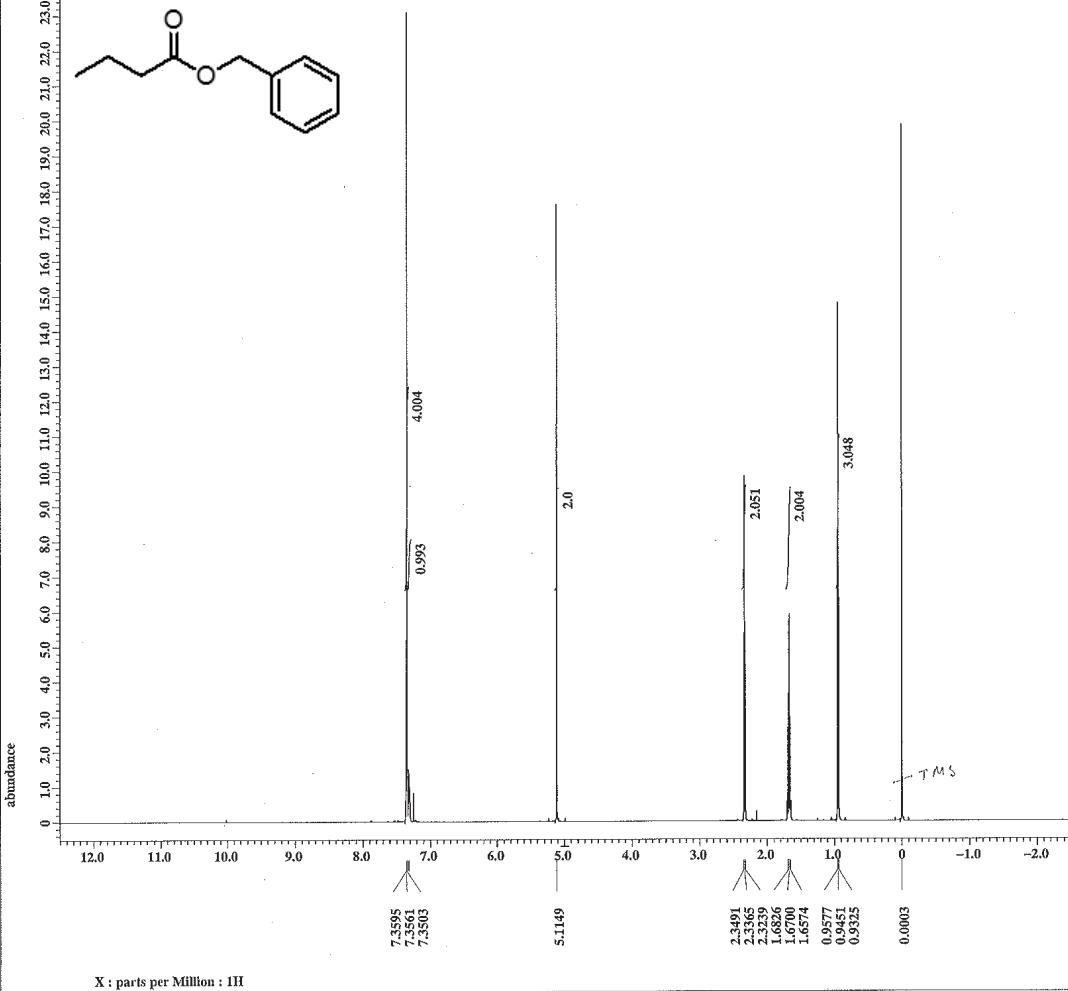
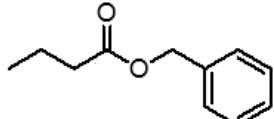
¹H NMR (600.17 MHz, CDCl₃, TMS): δ 8.0 (d, *J* = 8.94 Hz, 2H), 6.91 (d, *J* = 8.94 Hz, 2H), 4.24 (t, *J* = 6.84 Hz, 2H), 3.85 (s, 3H), 1.80-1.75(m, 2H), 1.02 (t, *J* = 7.56 Hz, 3H); ¹³C NMR (150.92 MHz, CDCl₃) δ 166.46, 163.25, 131.54 (C×2), 122.97, 113.56 (C×2), 66.24, 55.40, 22.18, 10.55; GC-MS m/e 194.095.

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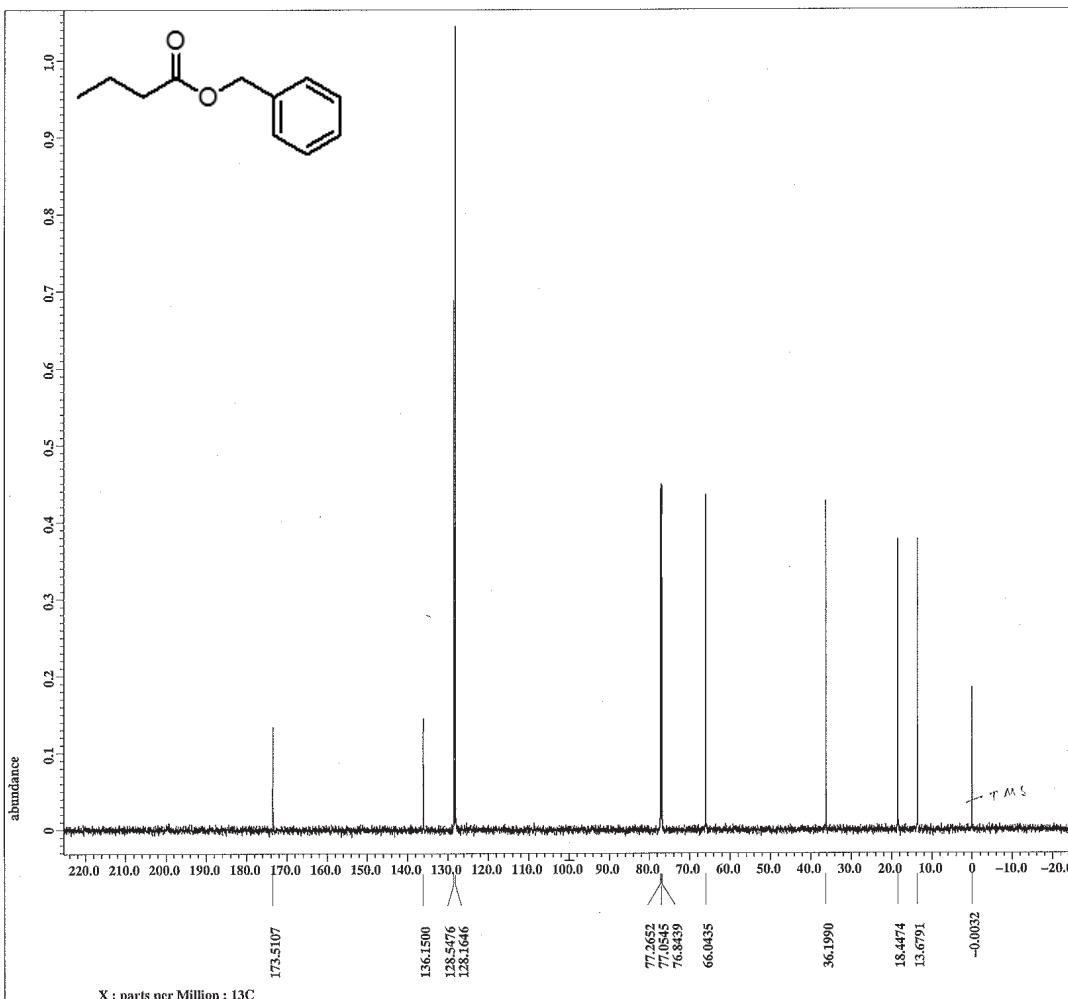
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x_pulse     = 6.5[us]
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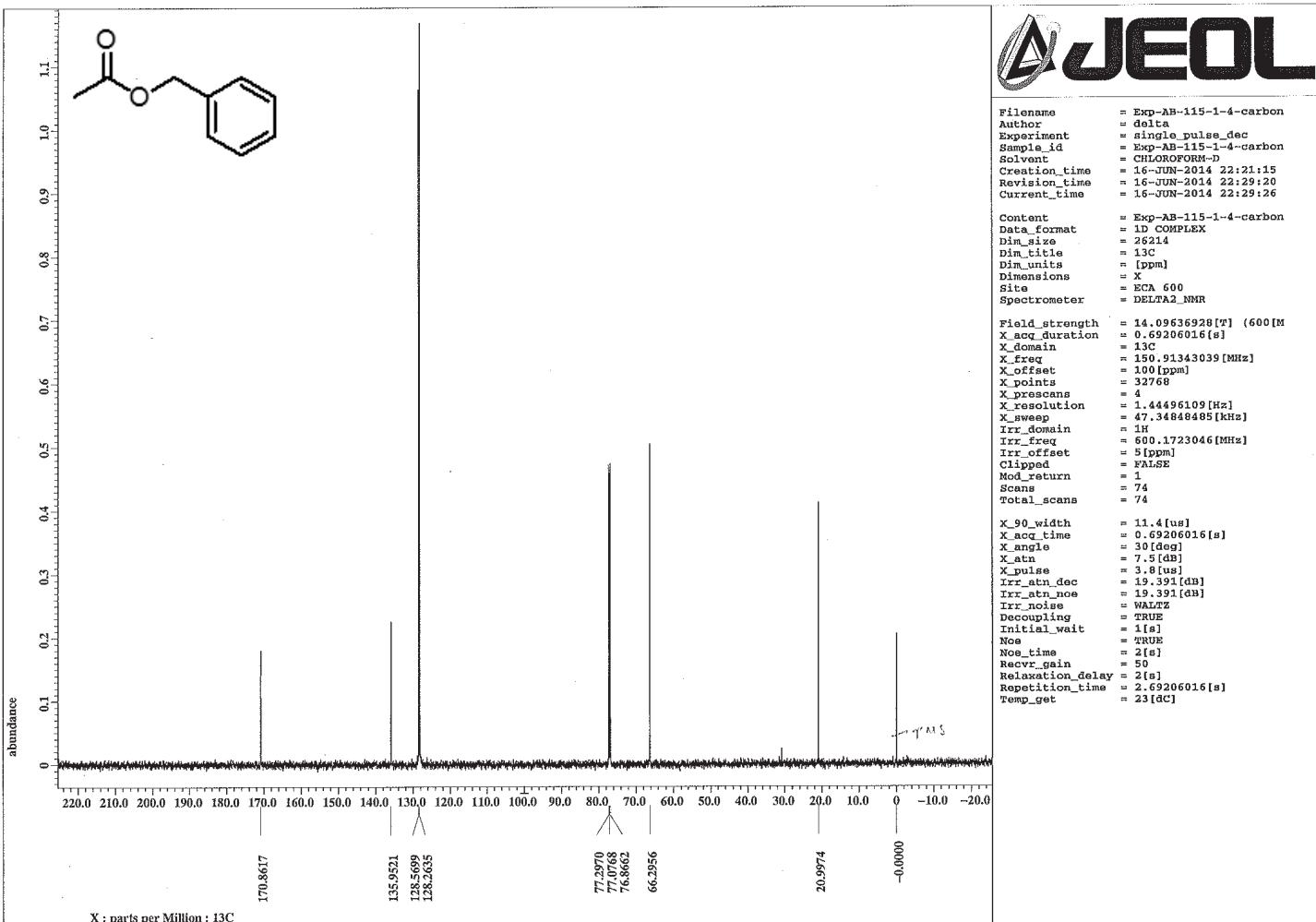
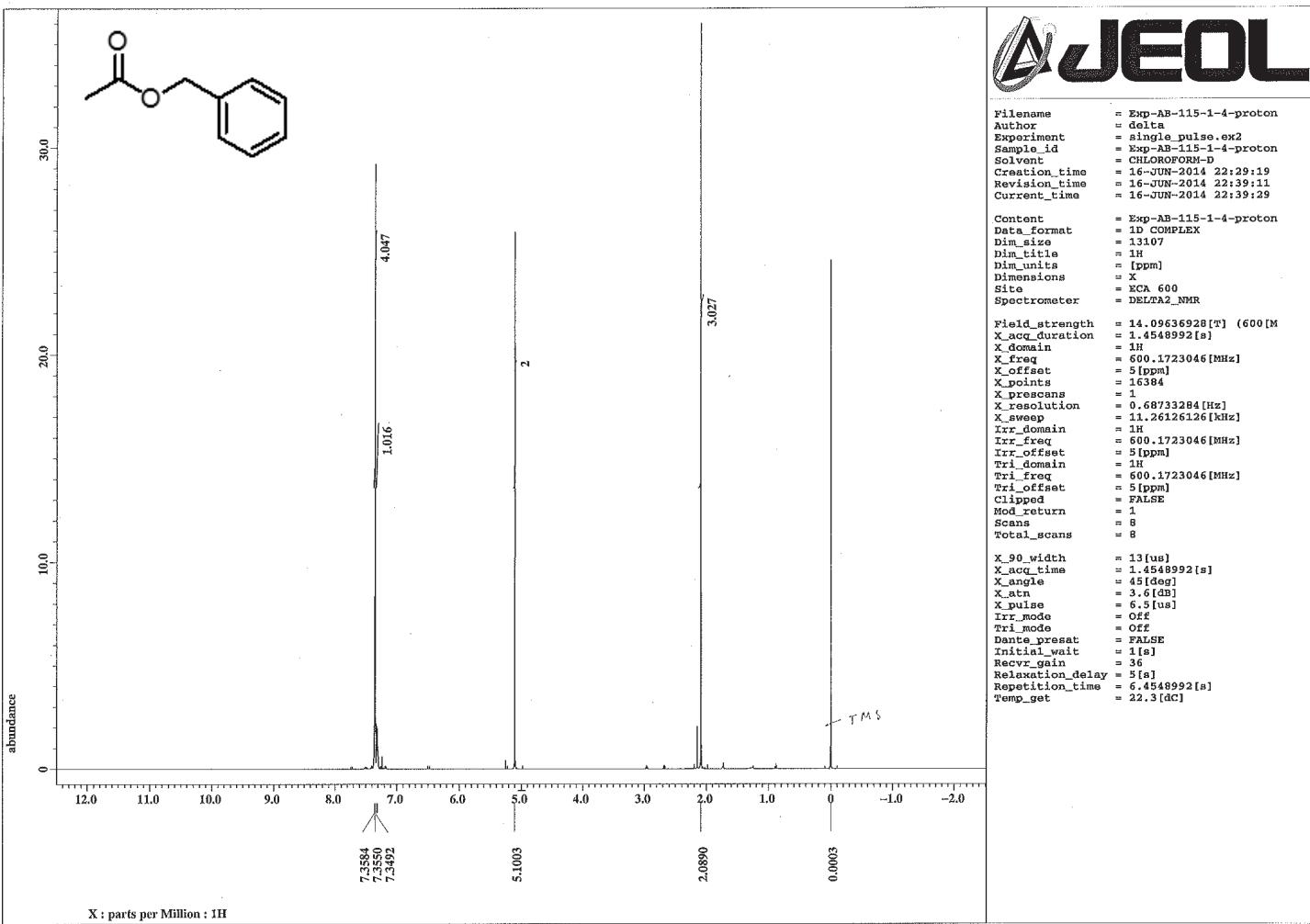
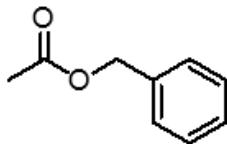
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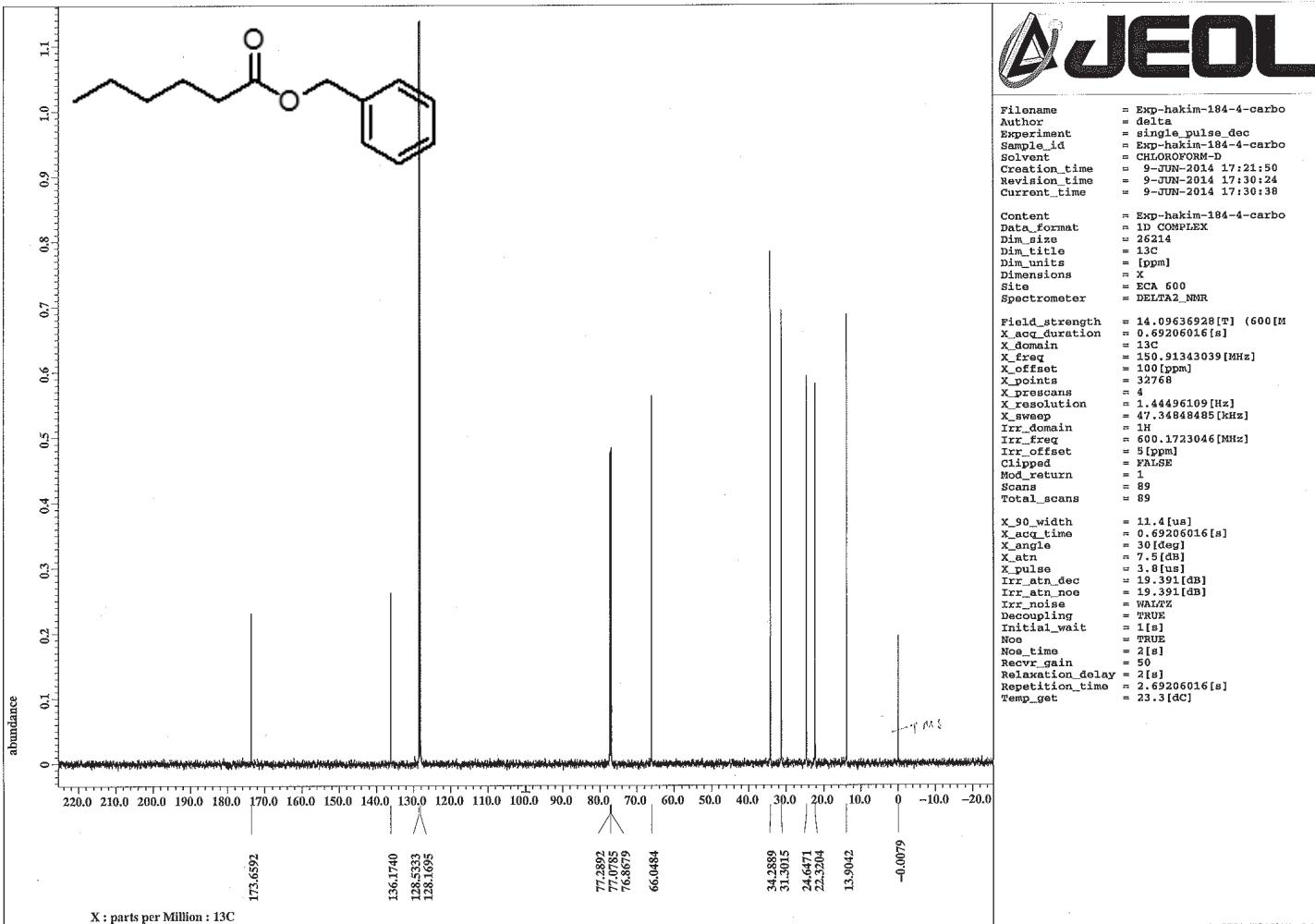
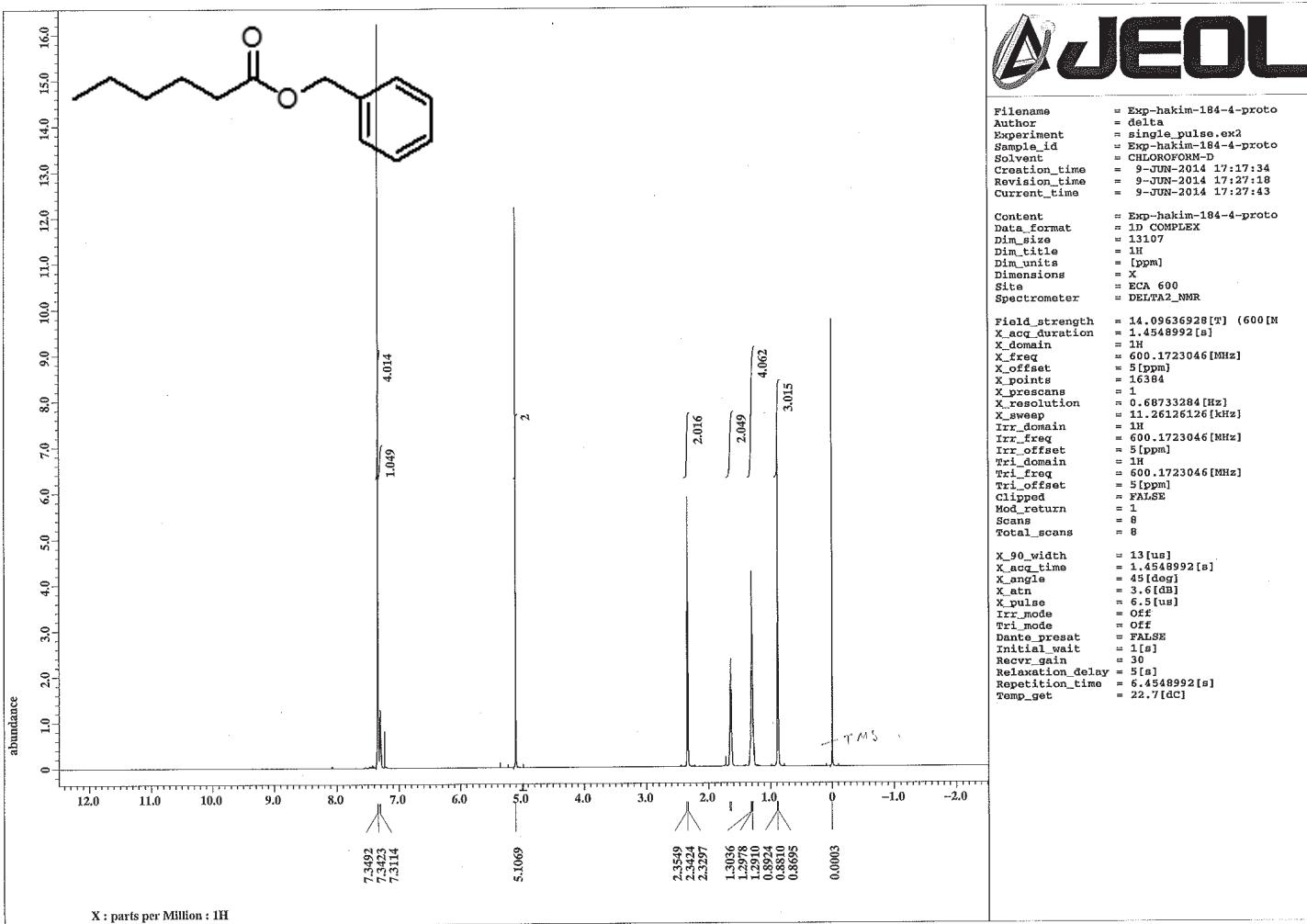
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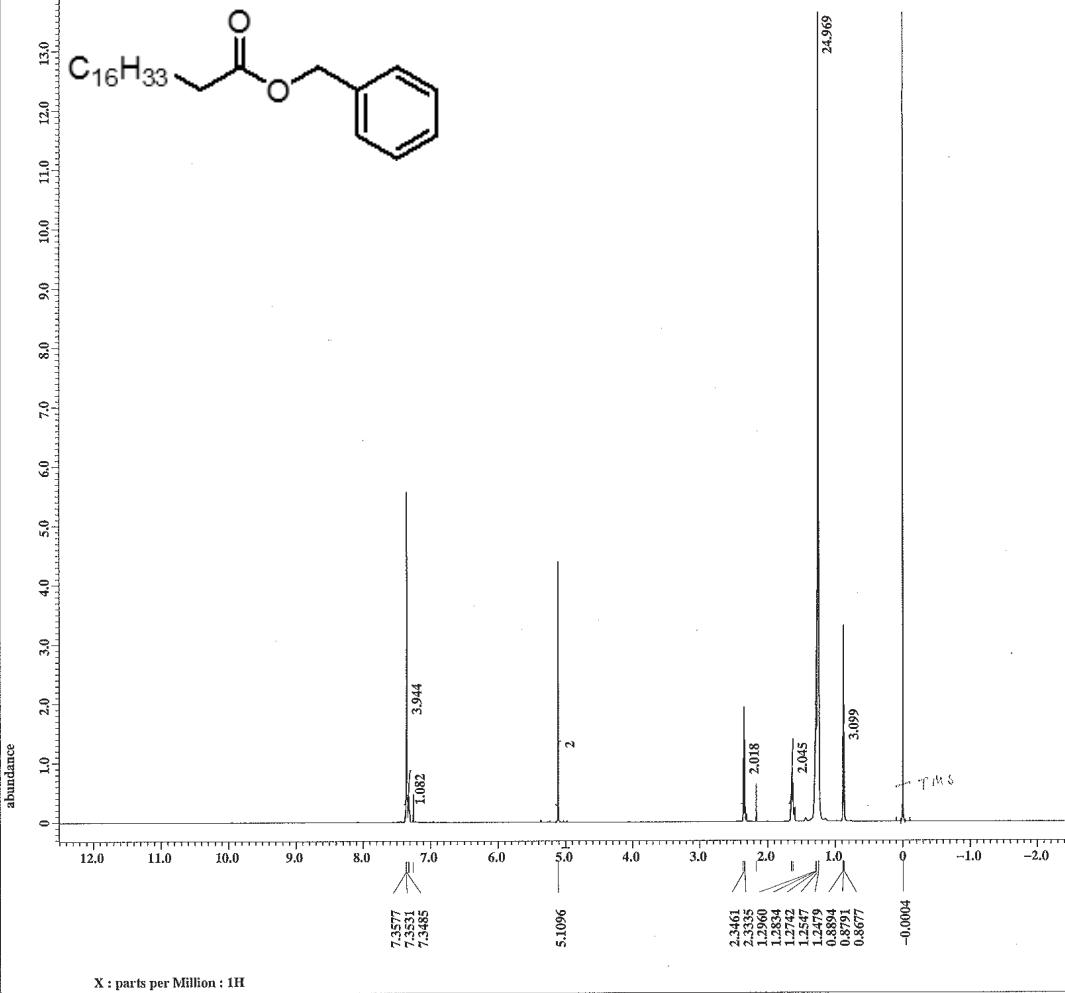
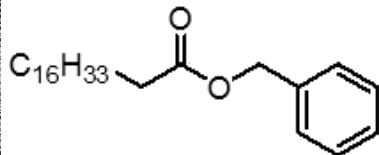
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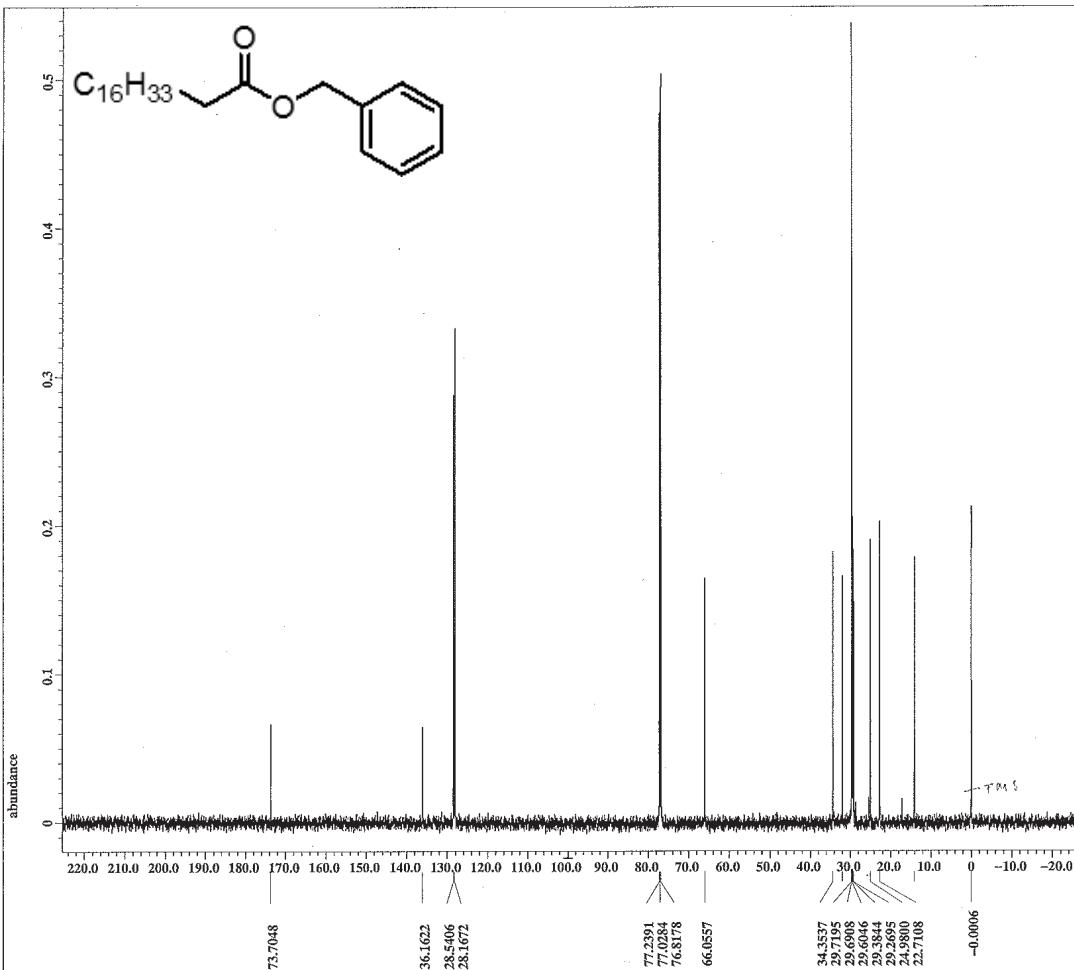
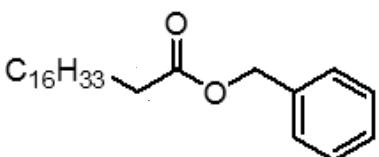
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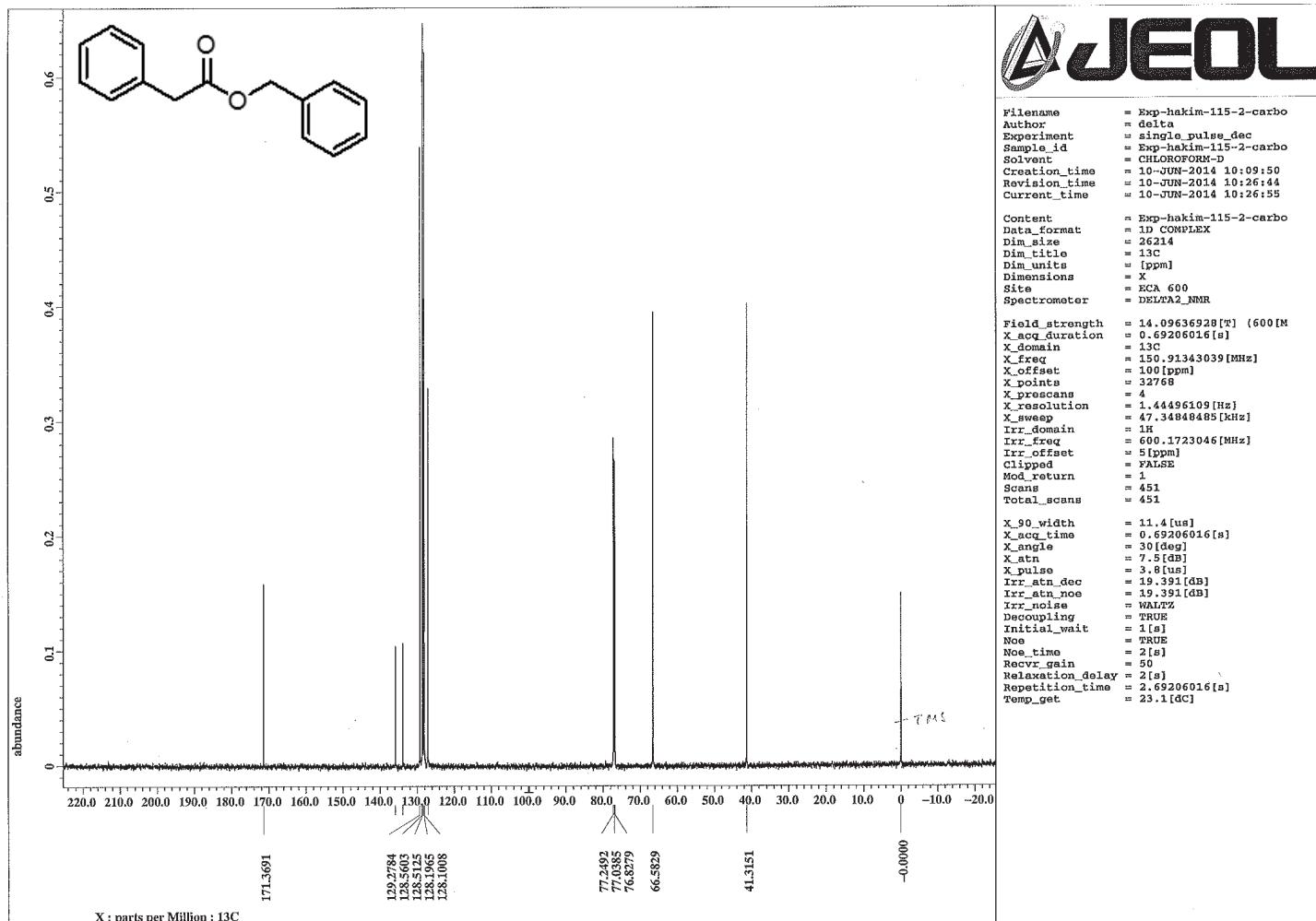
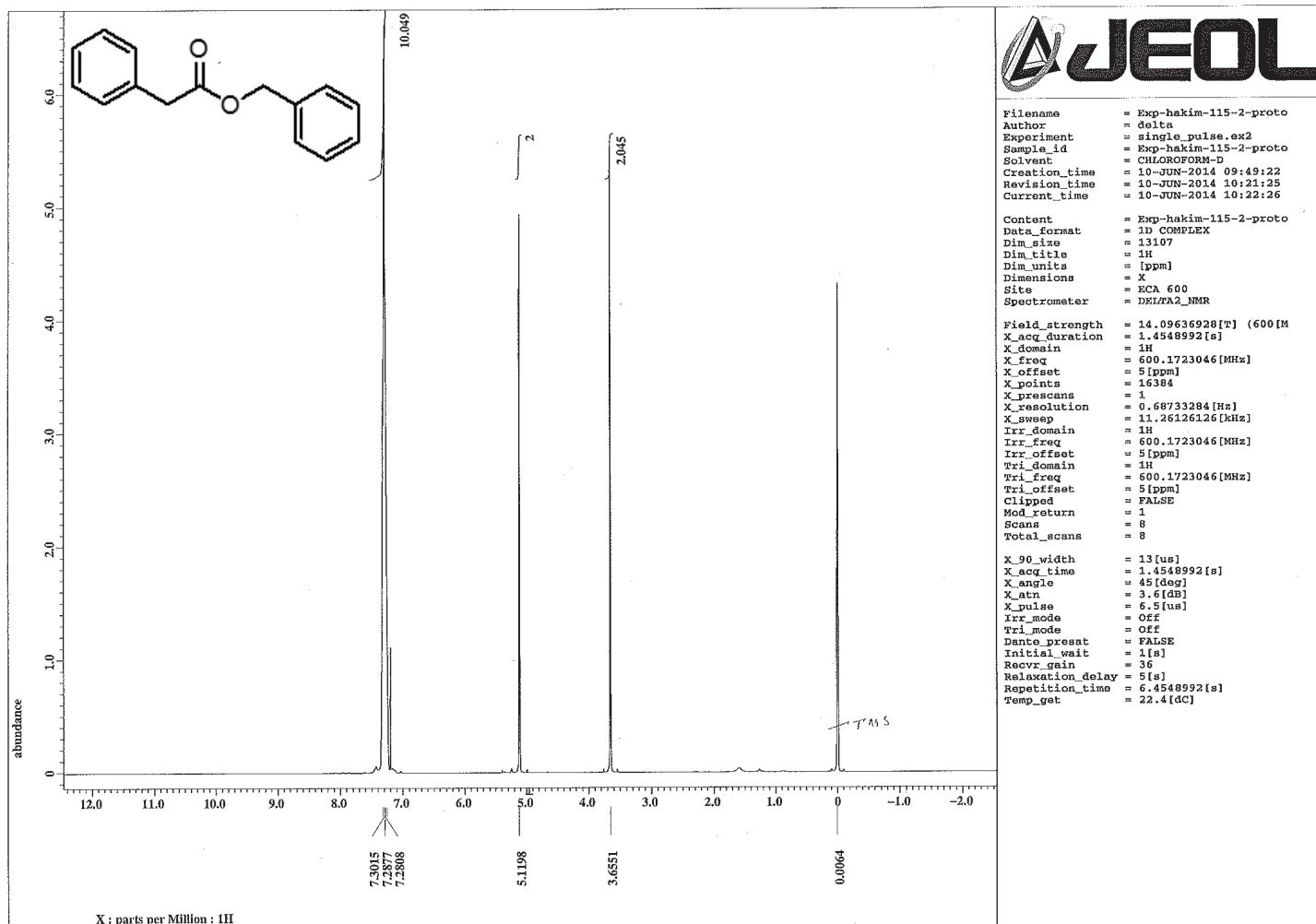
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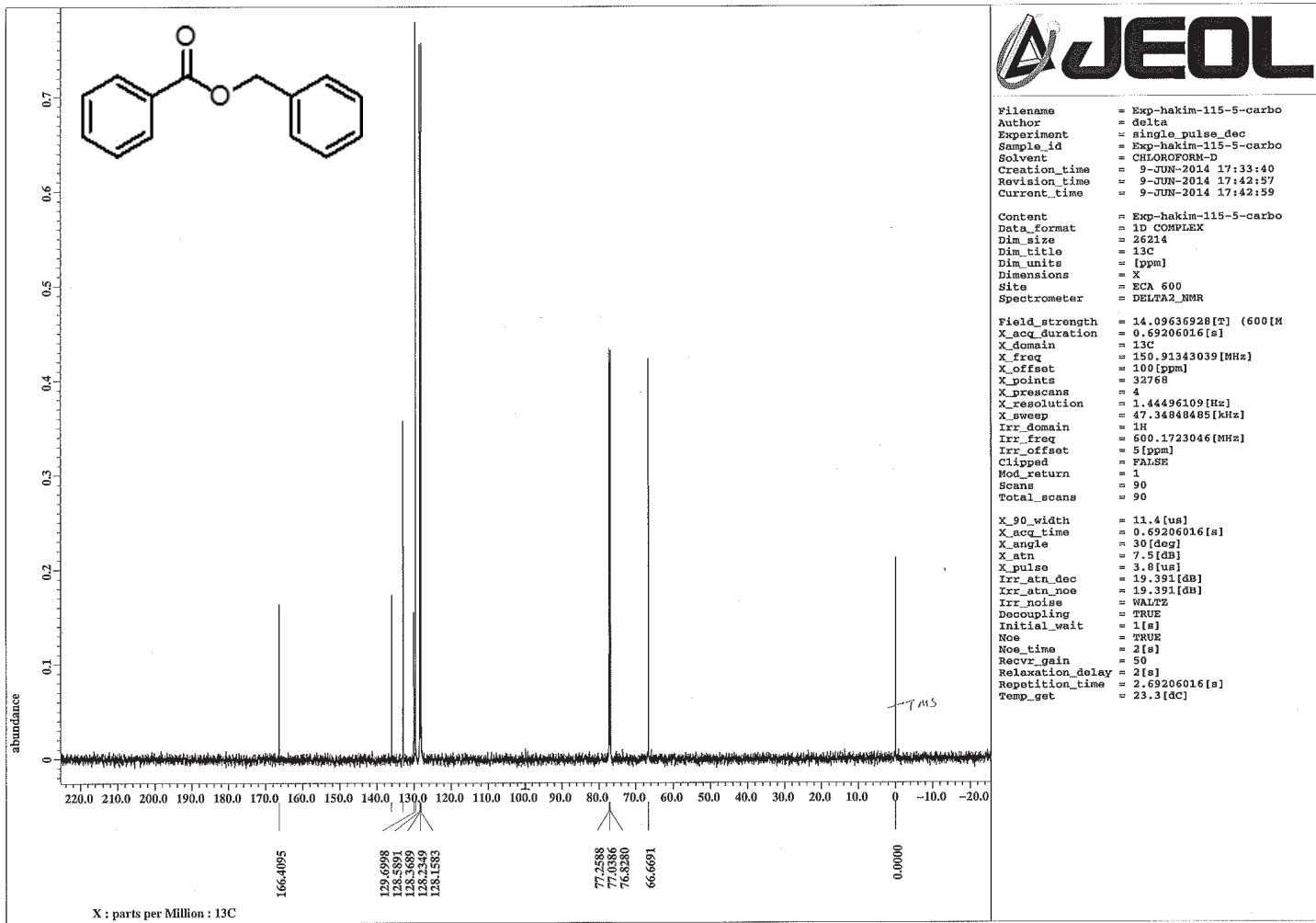
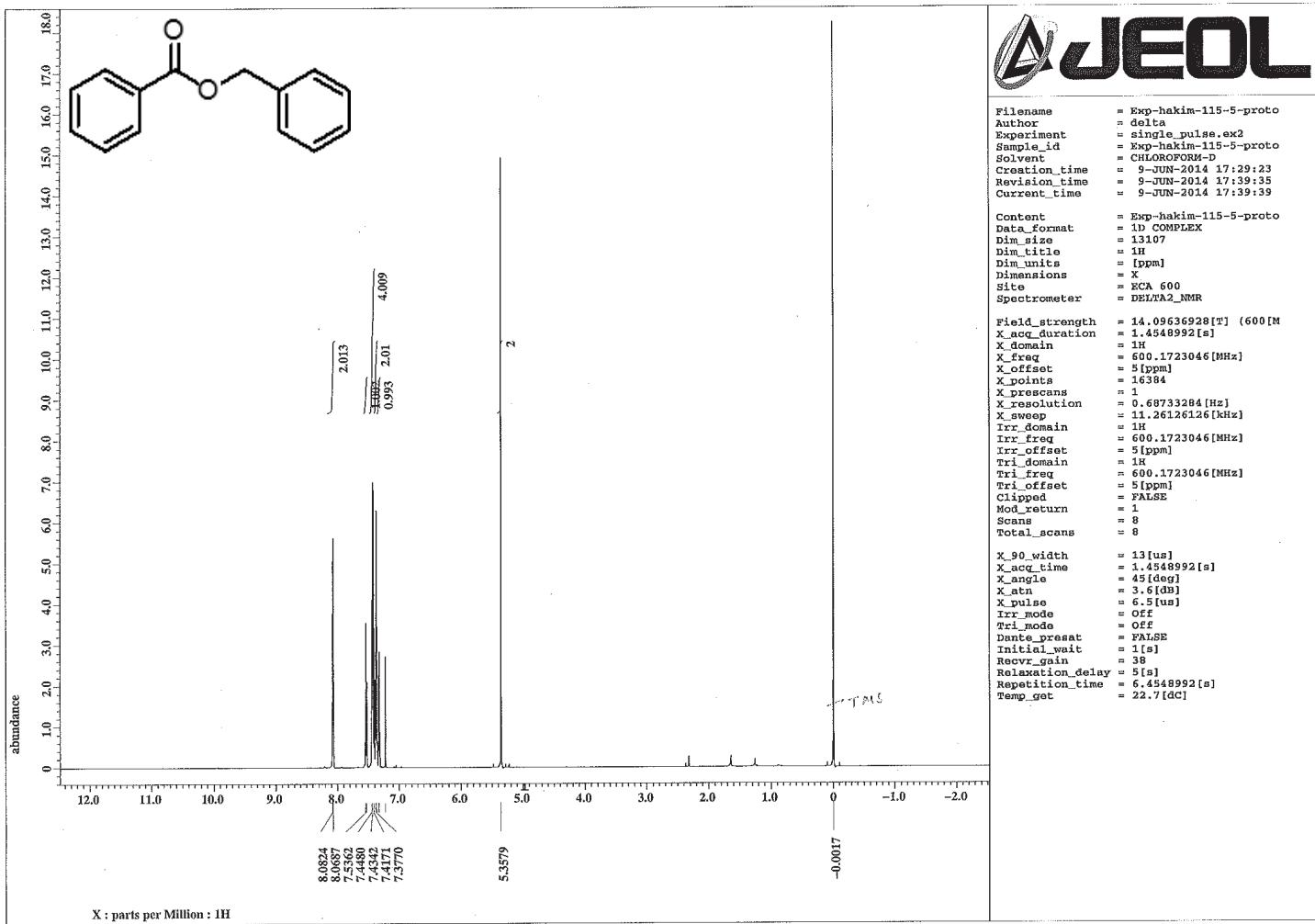
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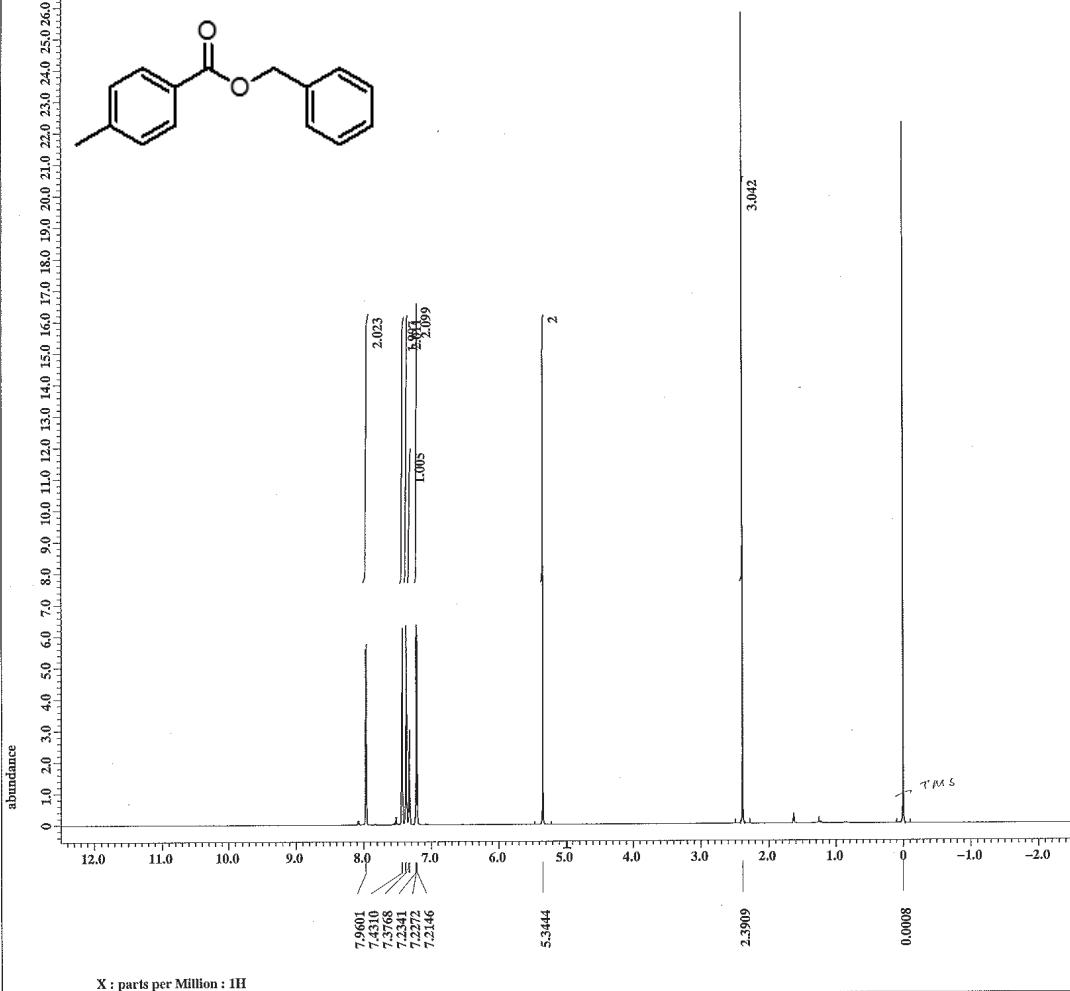
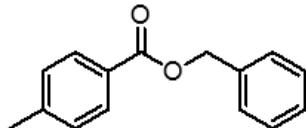
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X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.5[db]
X_pulse = 3.8[us]
Irr_atn_dec = 19.391[db]
Irr_atn_noe = 19.391[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Rwv_min = 5[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get = 23.4[dC]

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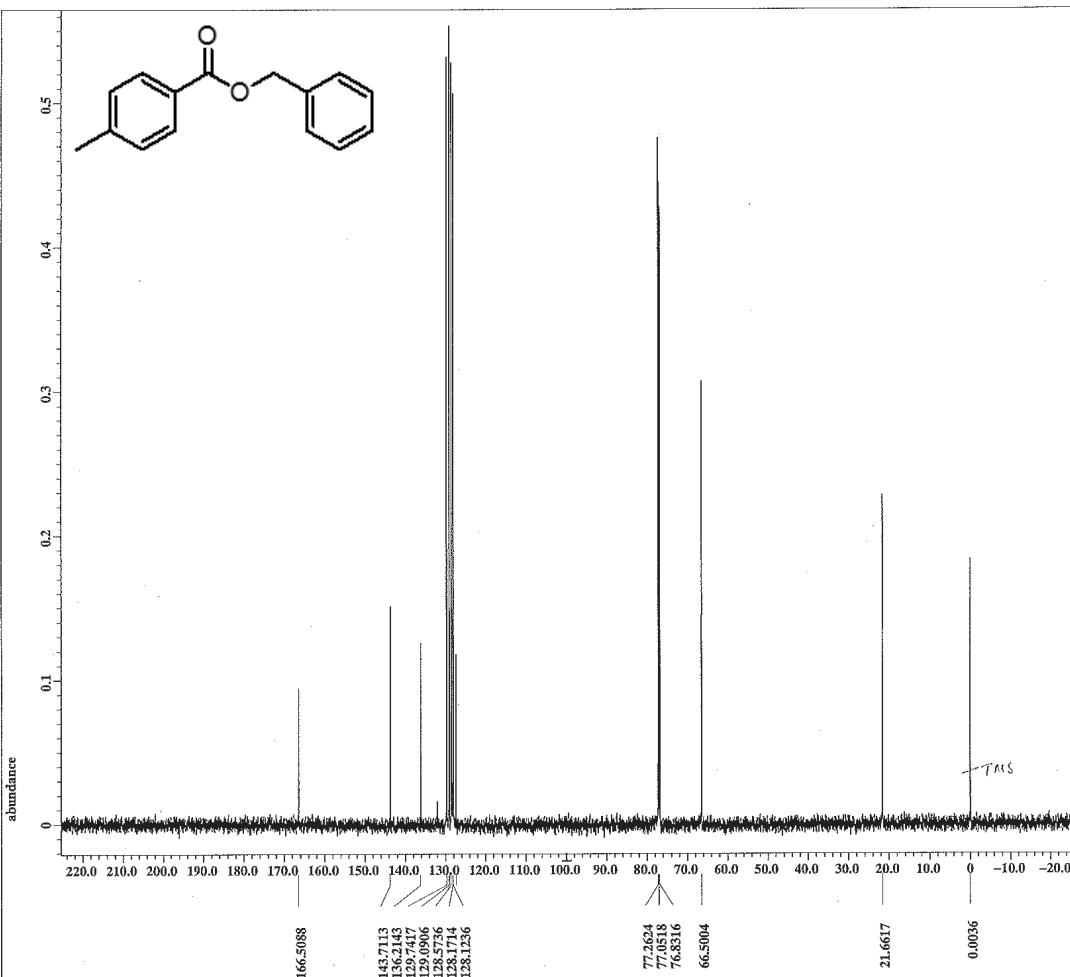
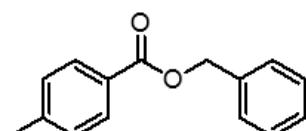
filename = Exp-hakim-115-9-proto
author = delta
Experiment = single_pulse.ex2
Sample_id = Exp-hakim-115-9-proto
Solvant = CHLOROFORM-D
Creation_time = 9-JUN-2014 17:41:02
Revision_time = 9-JUN-2014 17:52:13
Current_time = 9-JUN-2014 17:52:18

Content = Exp-hakim-115-9-proto
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DNMRAZ_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_aver = 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[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Rw16_size = 4
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get = 22.7[dc]

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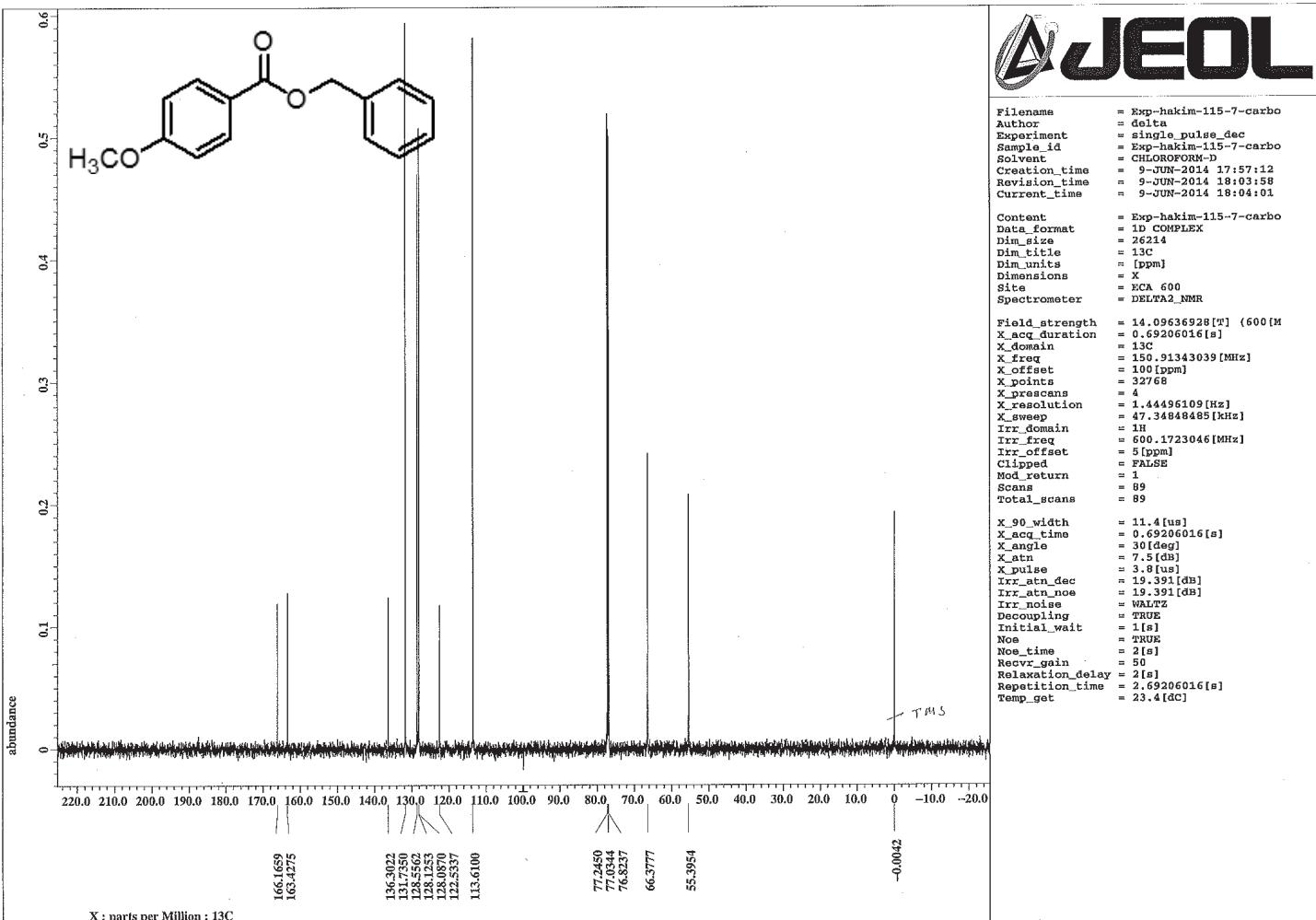
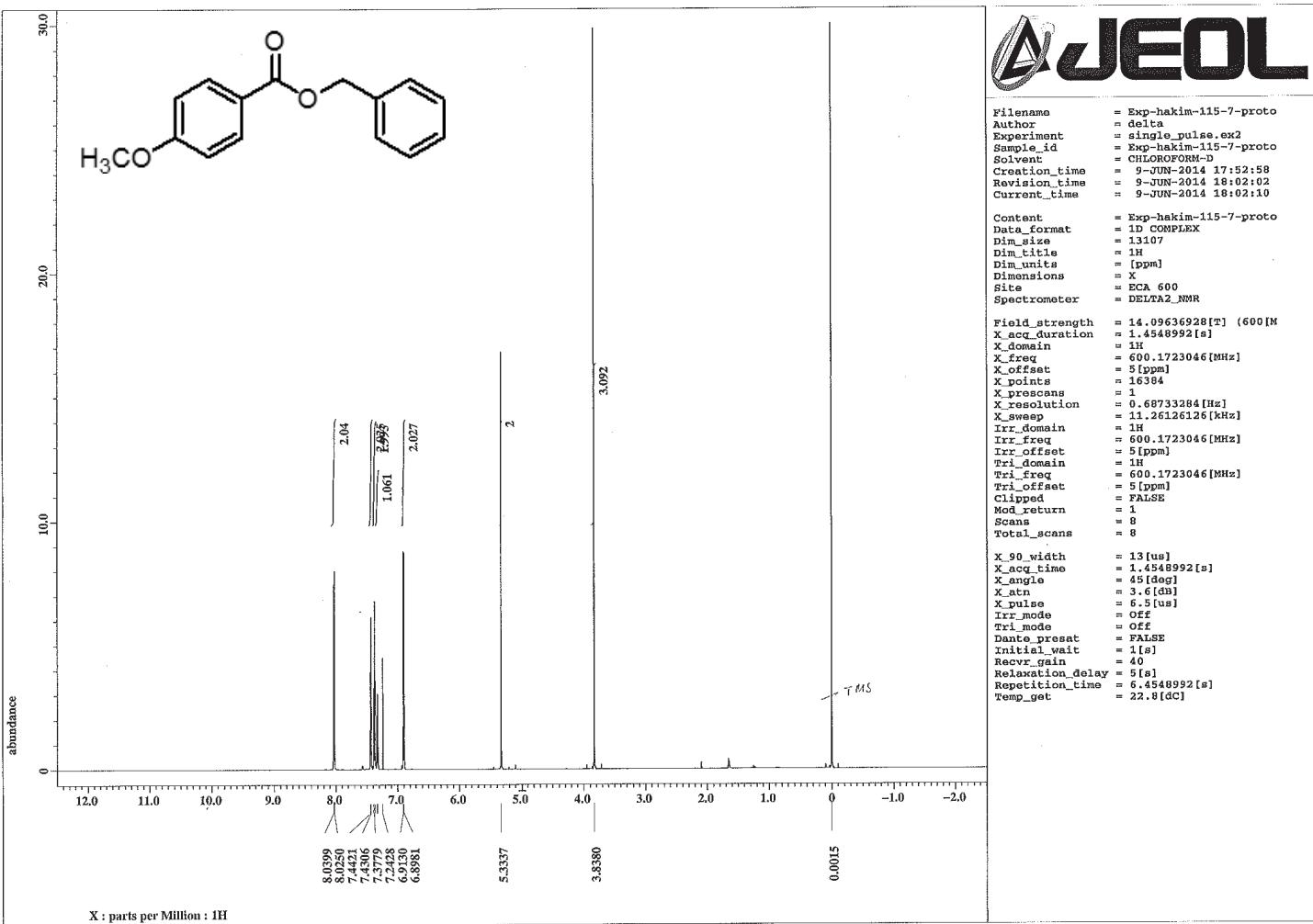
filename = Exp-hakim-115-9-carbo
author = delta
Experiment = single_pulse_dec
Sample_id = Exp-hakim-115-9-carbo
Solvant = CHLOROFORM-D
Creation_time = 9-JUN-2014 17:46:13
Revision_time = 9-JUN-2014 17:55:06
Current_time = 9-JUN-2014 17:55:08

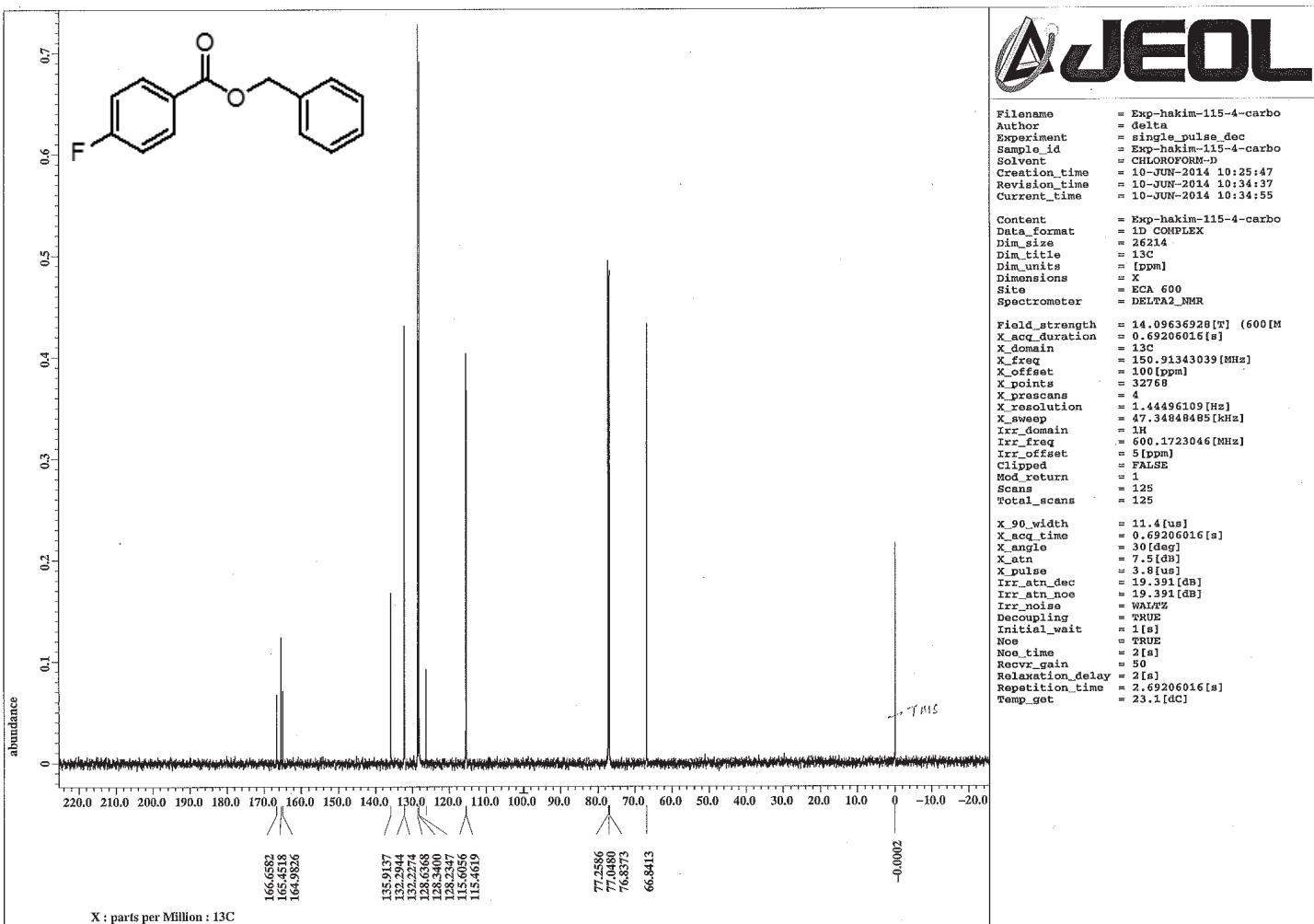
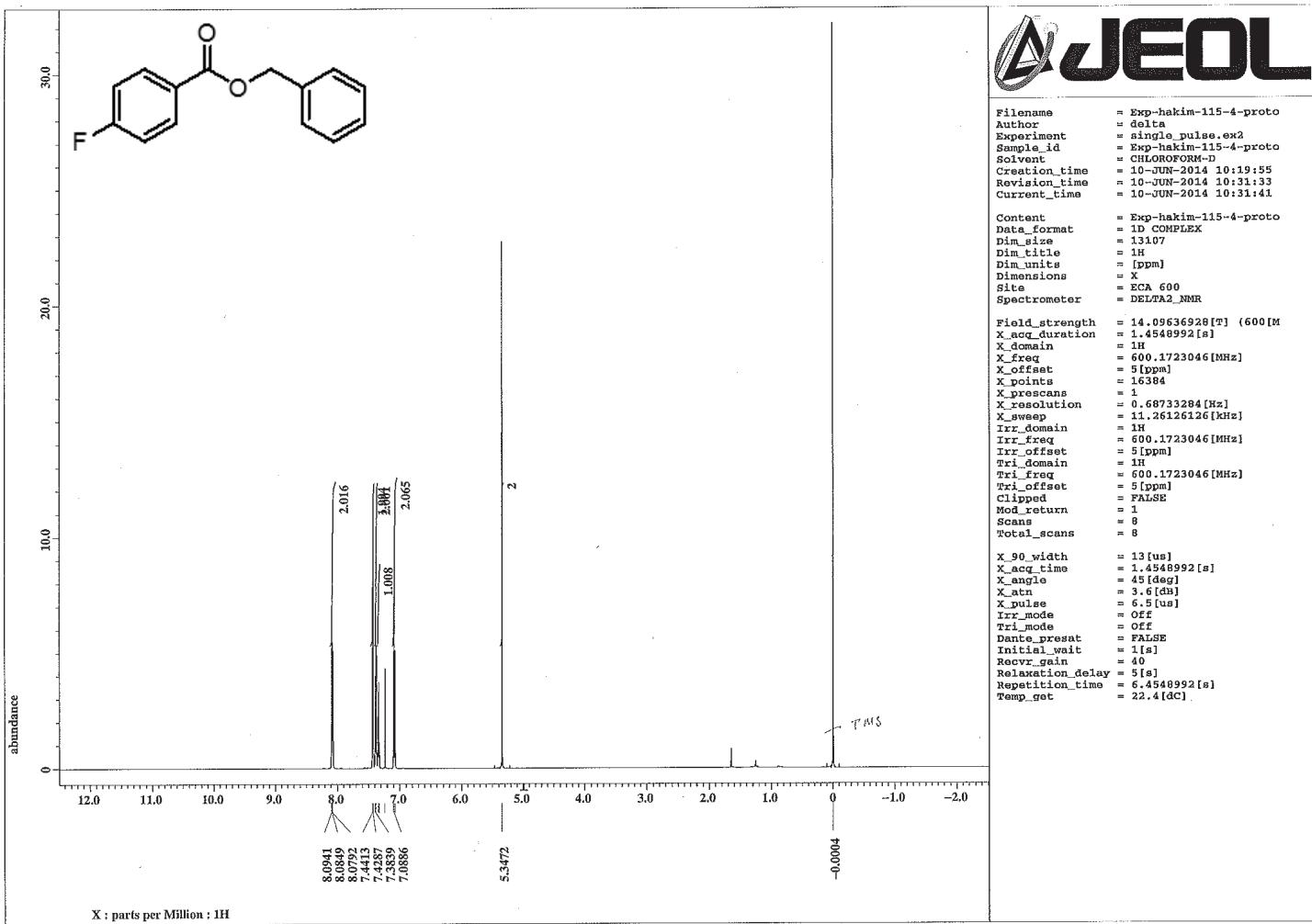
Content = Exp-hakim-115-9-carbo
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DNMRAZ_NMR

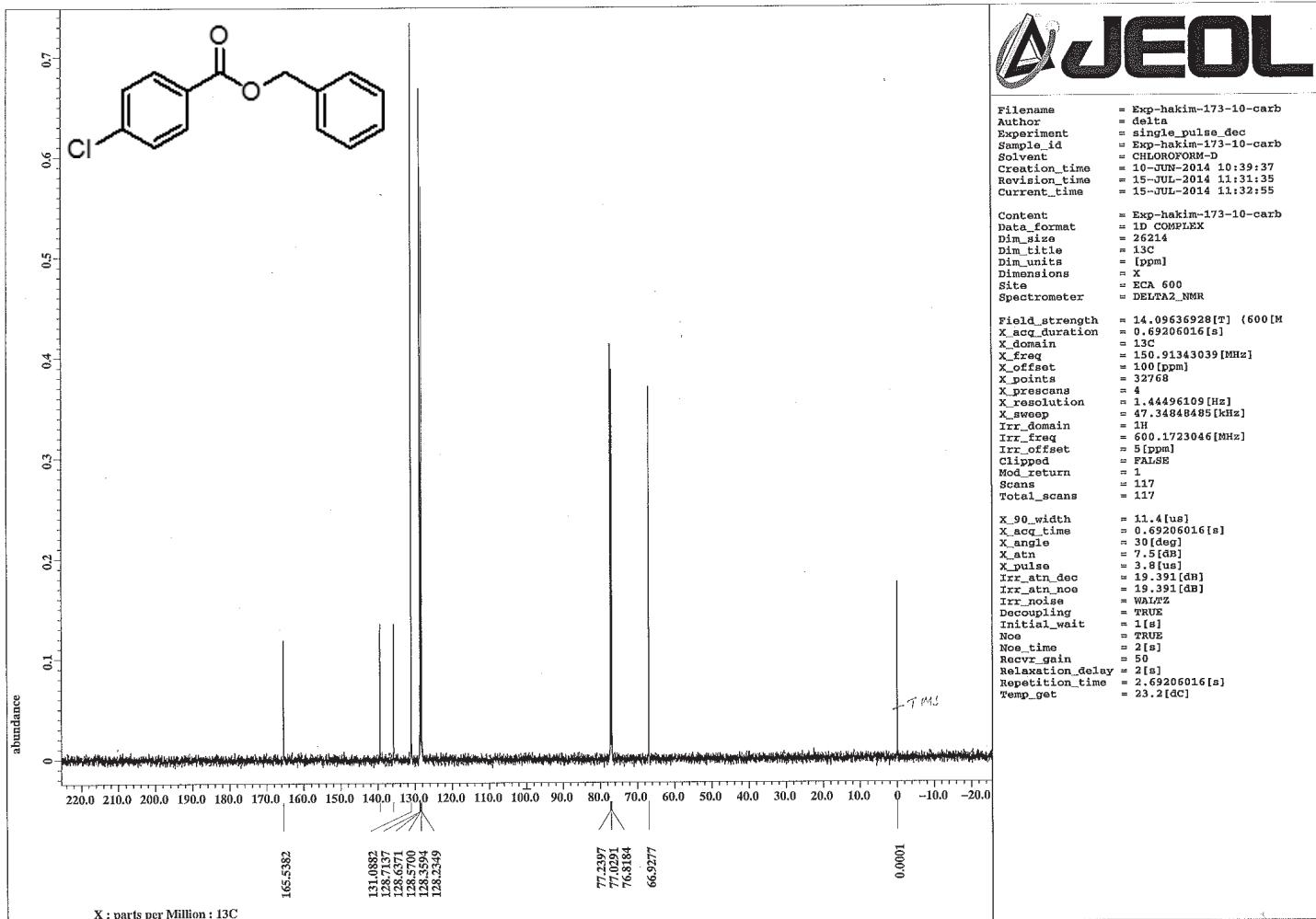
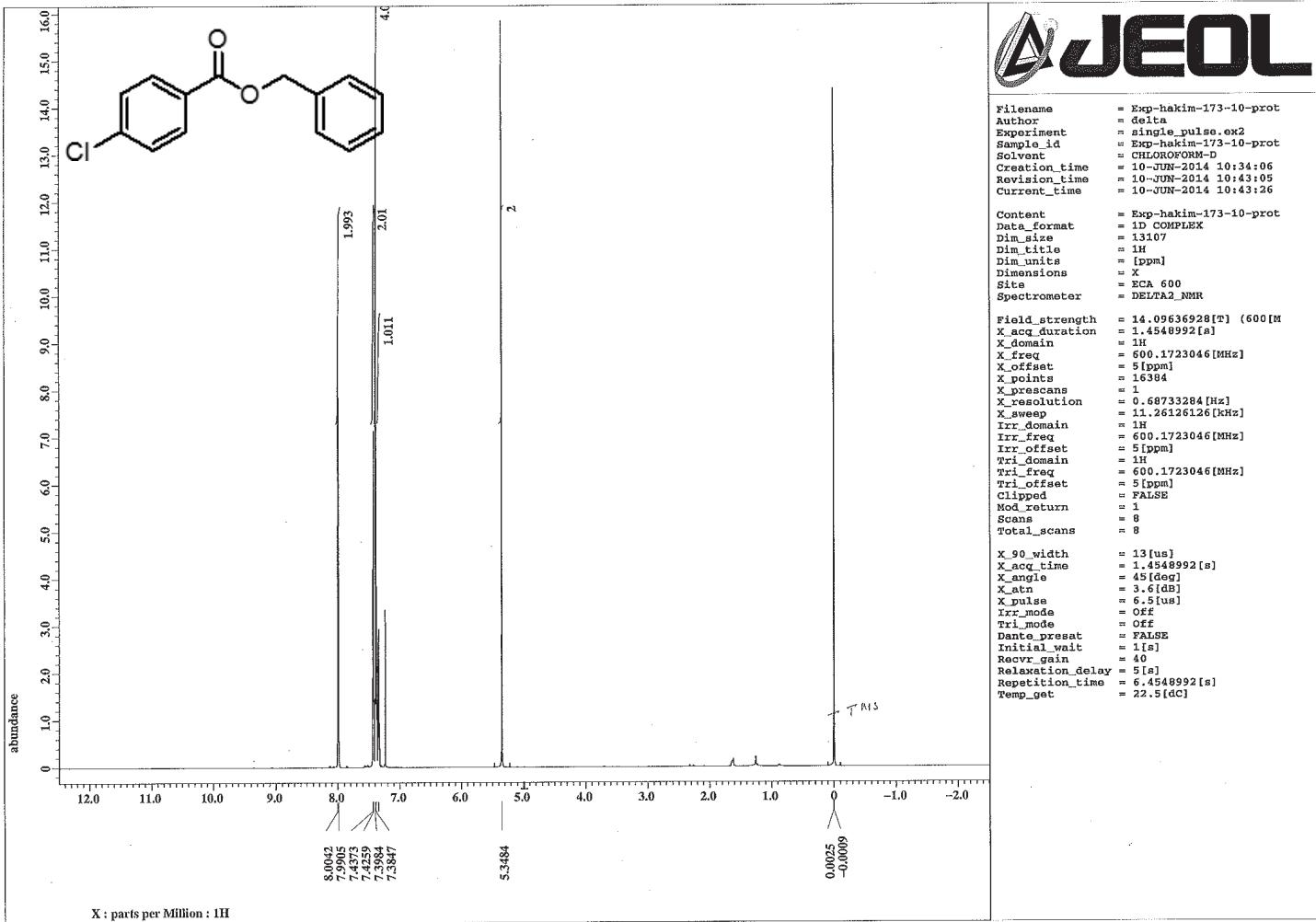
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_aver = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 110
Total_scans = 110

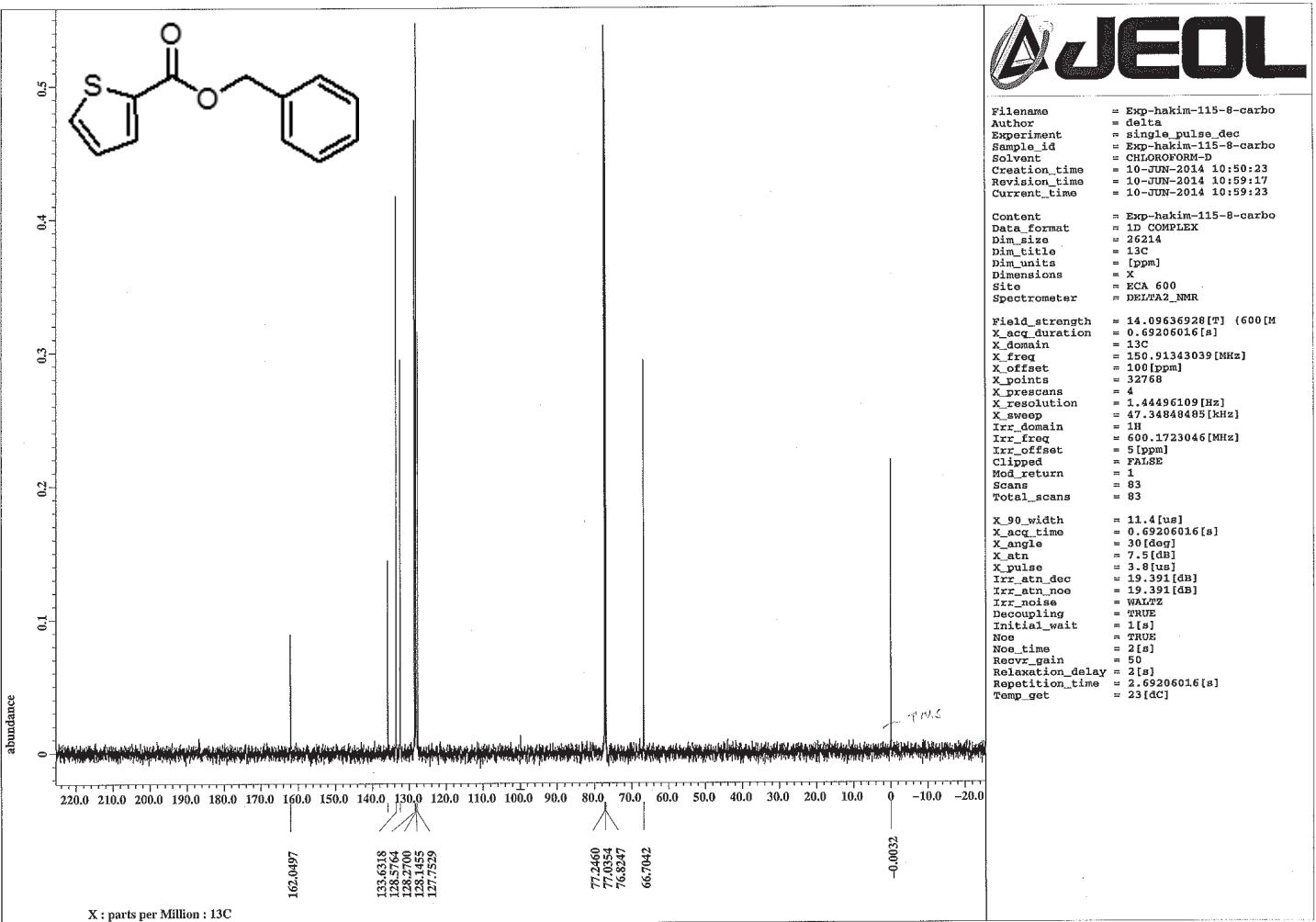
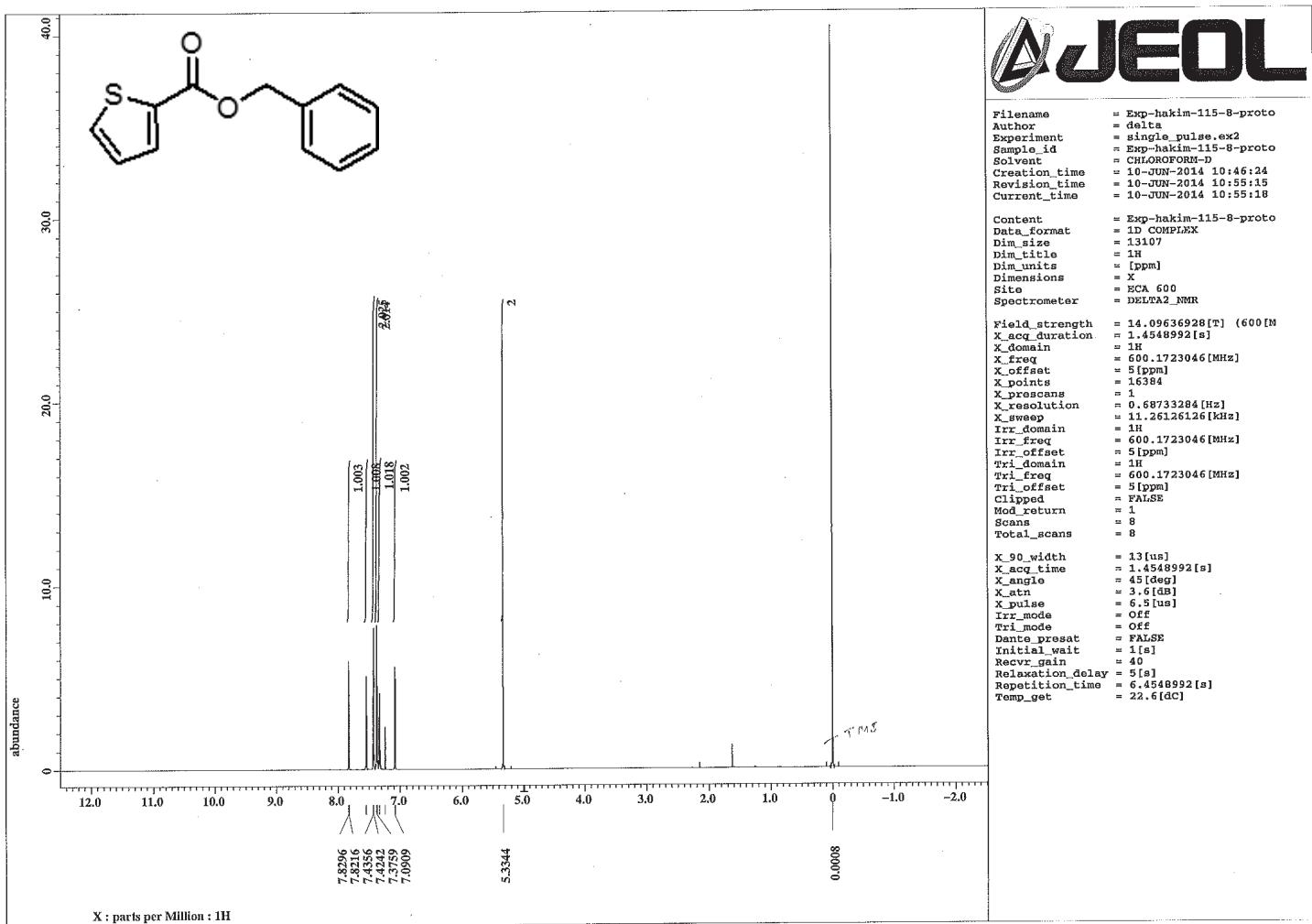
X_90_width = 11.4[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 3.8[us]
Irr_atn_dec = 19.391[db]
Irr_atn_noe = 19.391[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Noe_wait = 5[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get = 23.4[dc]

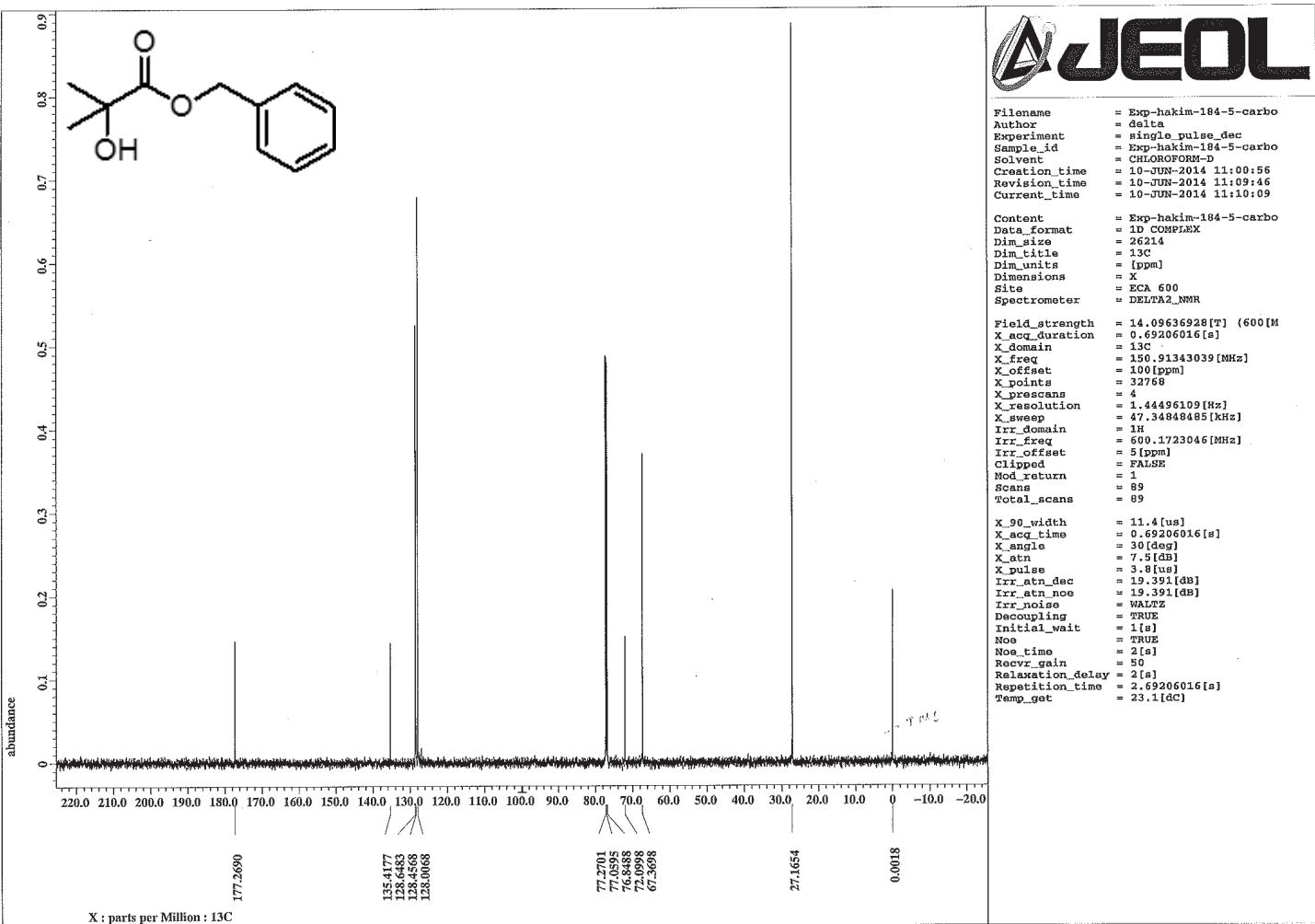
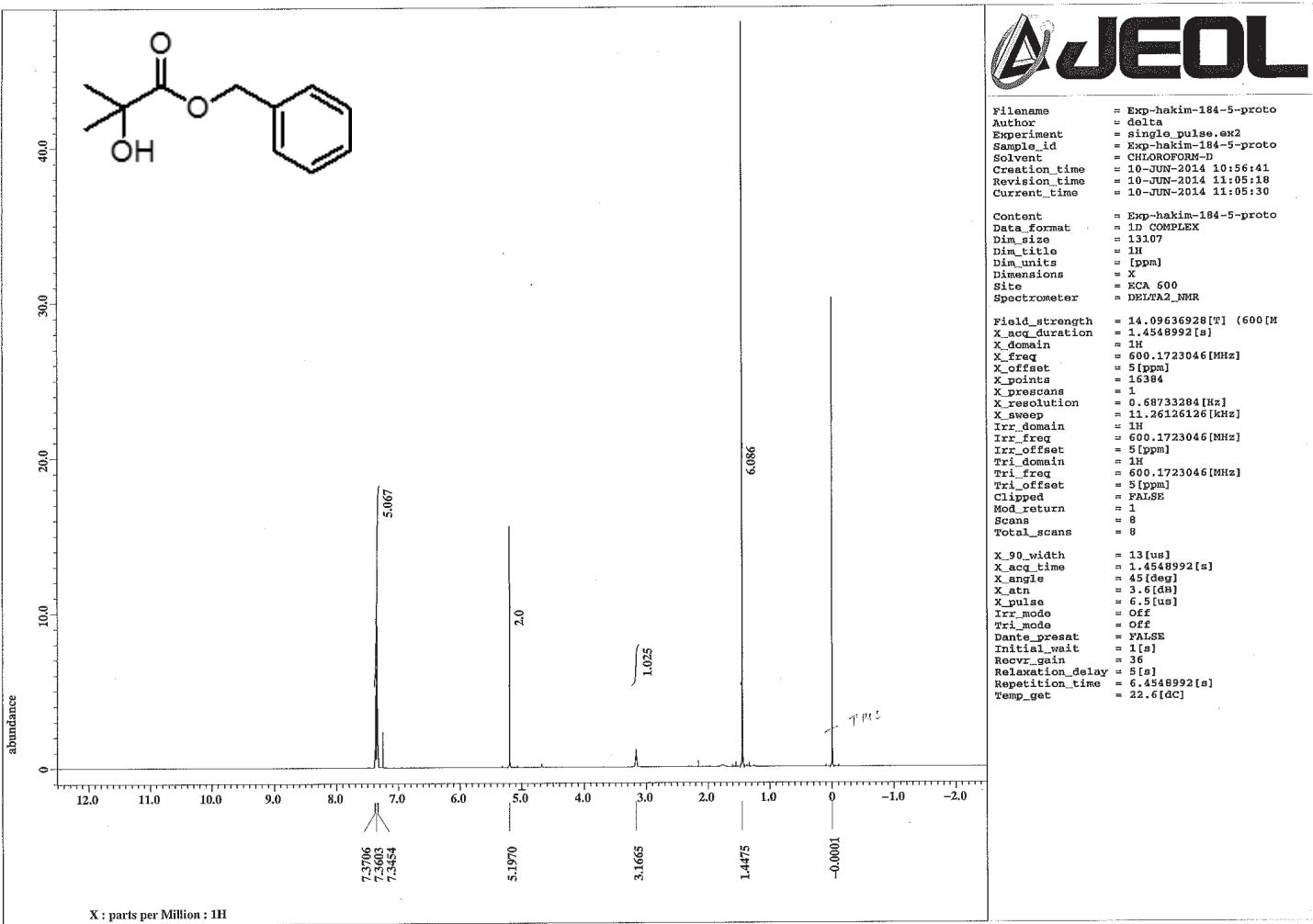
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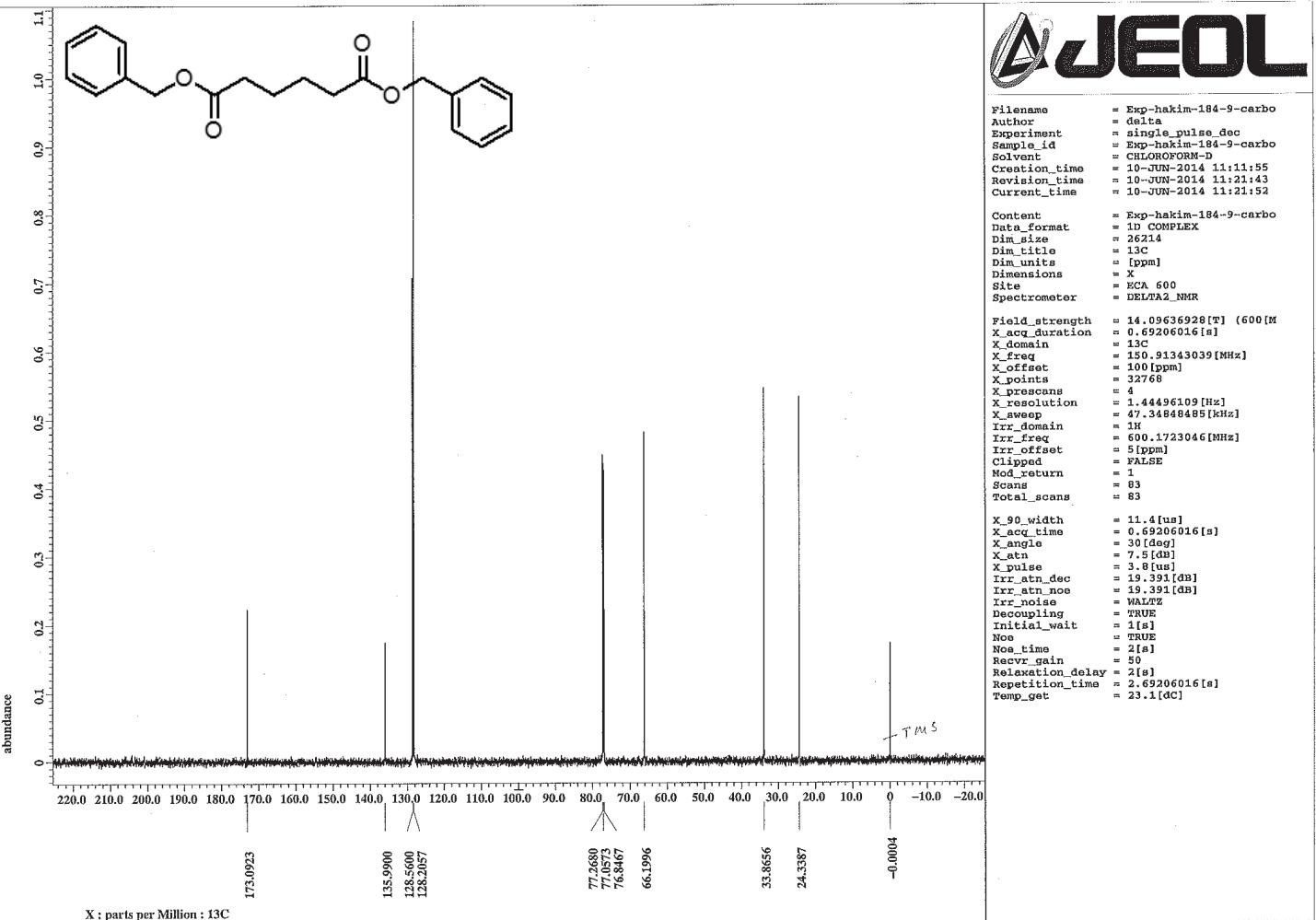
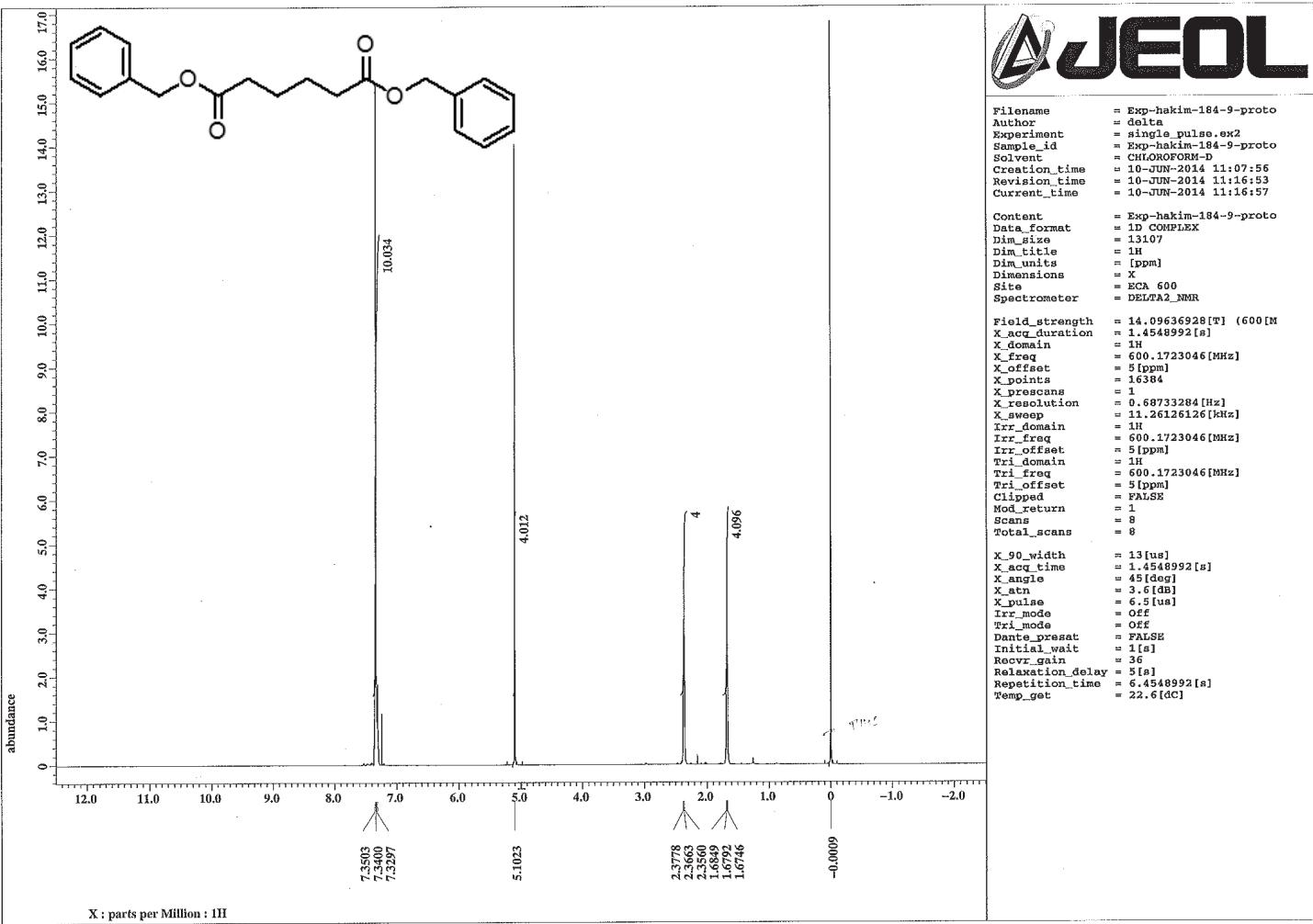


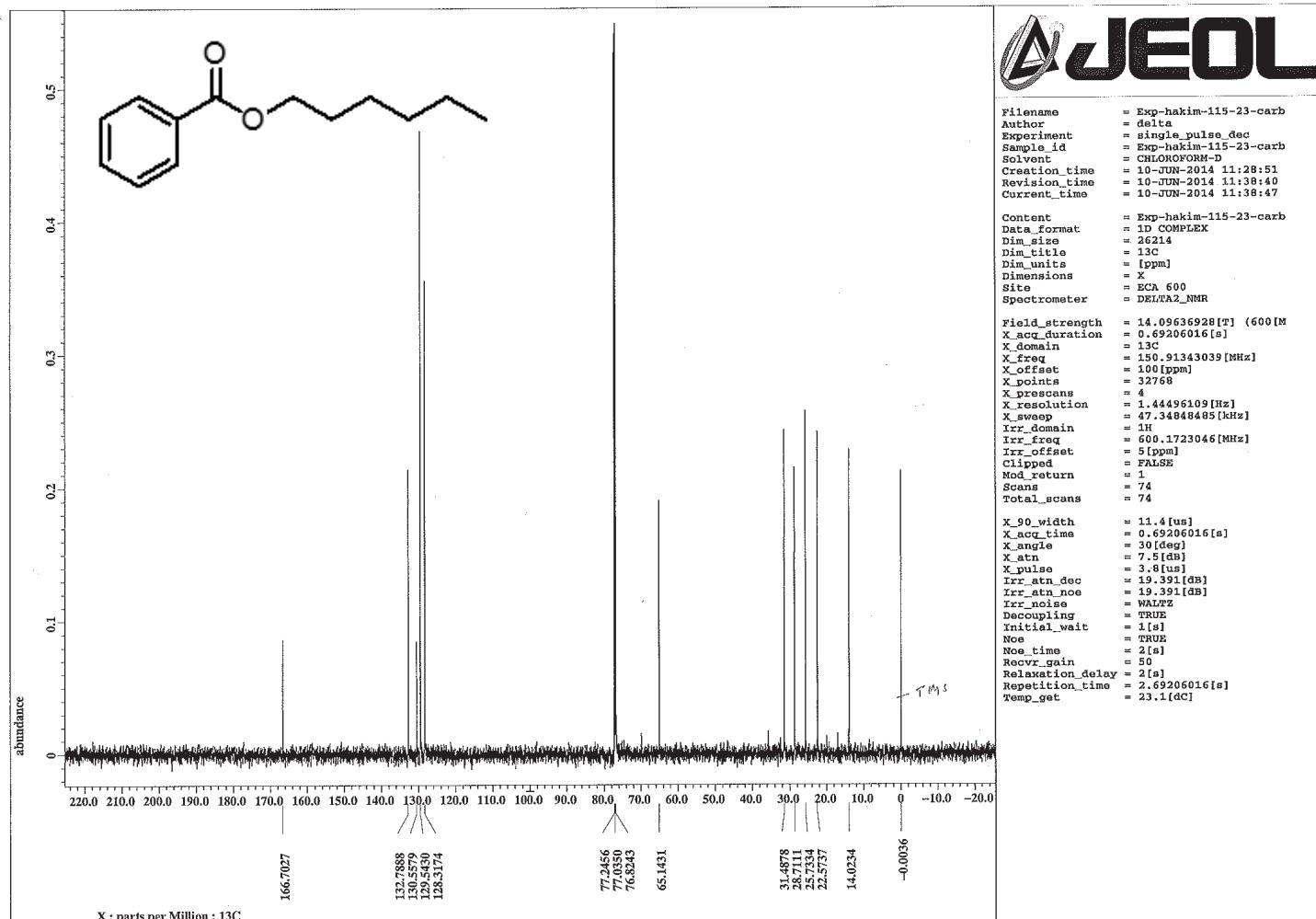
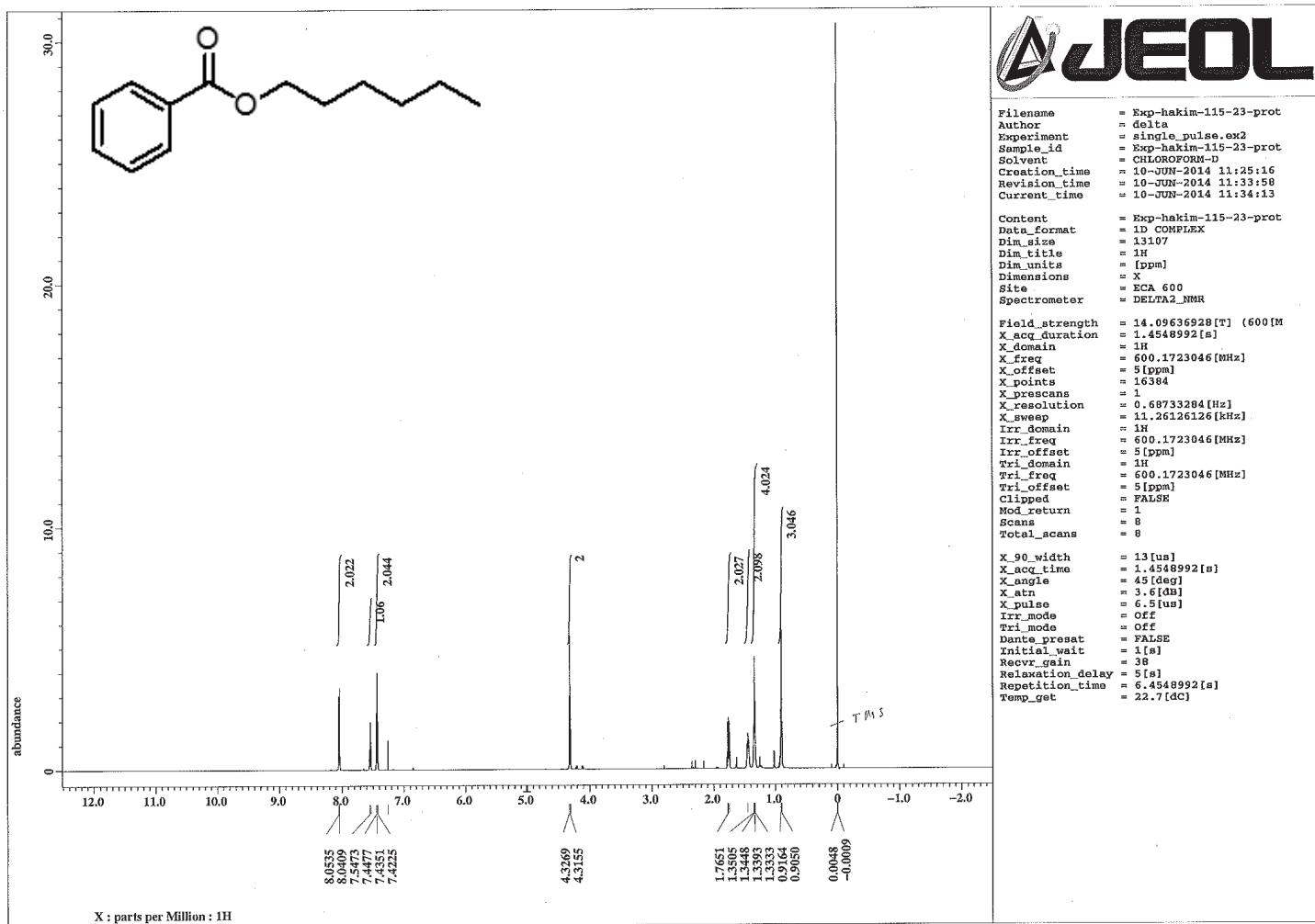


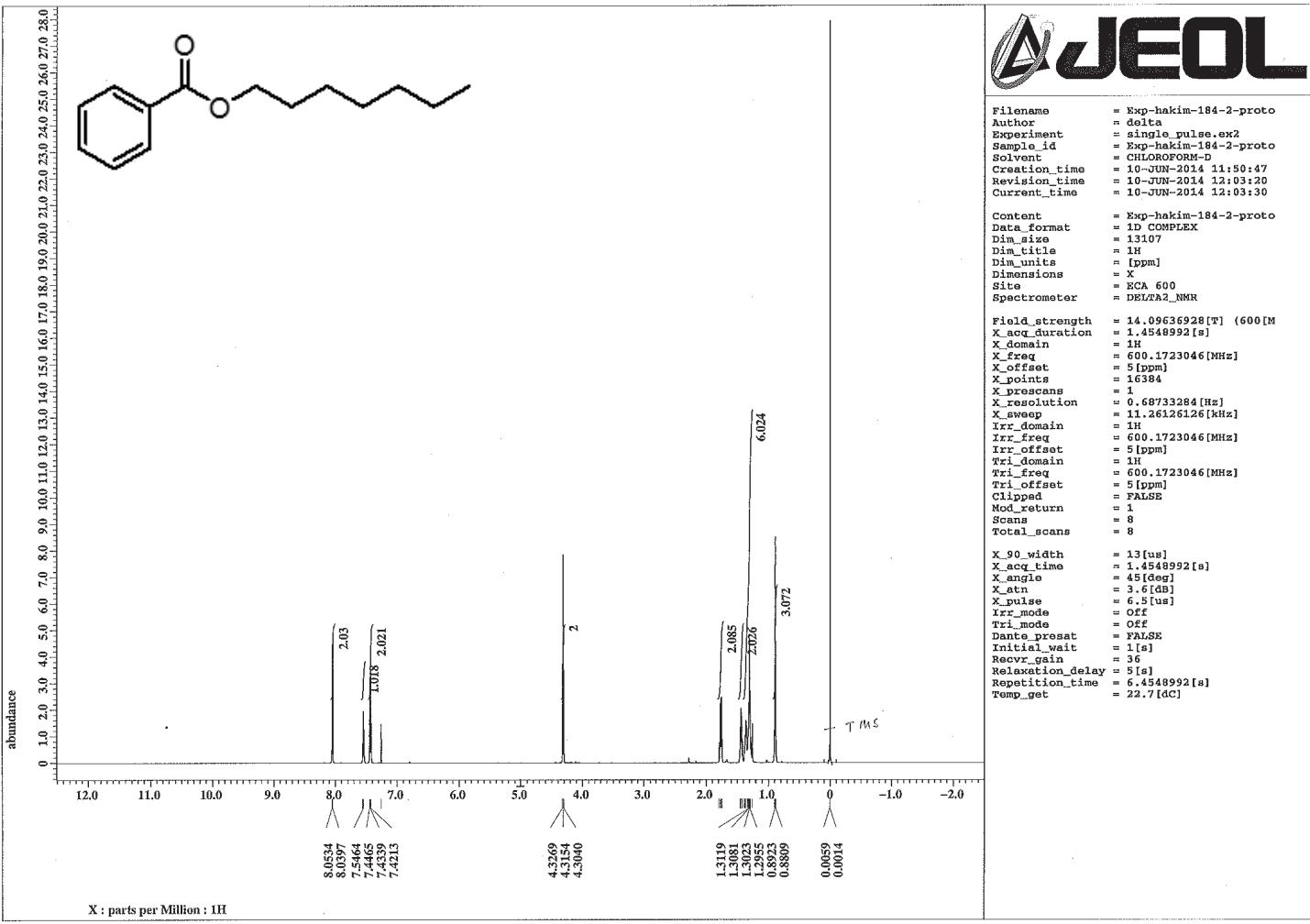


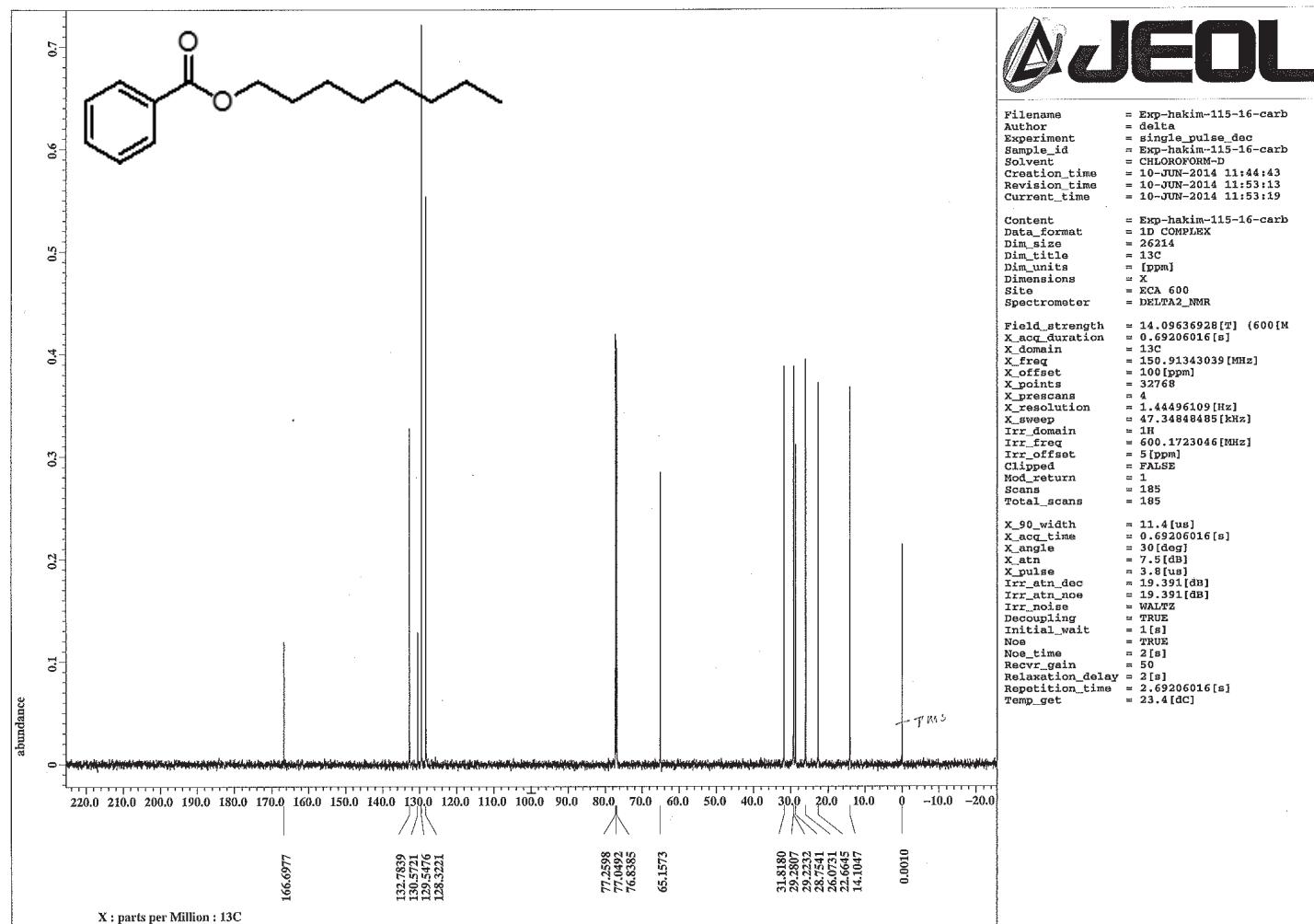
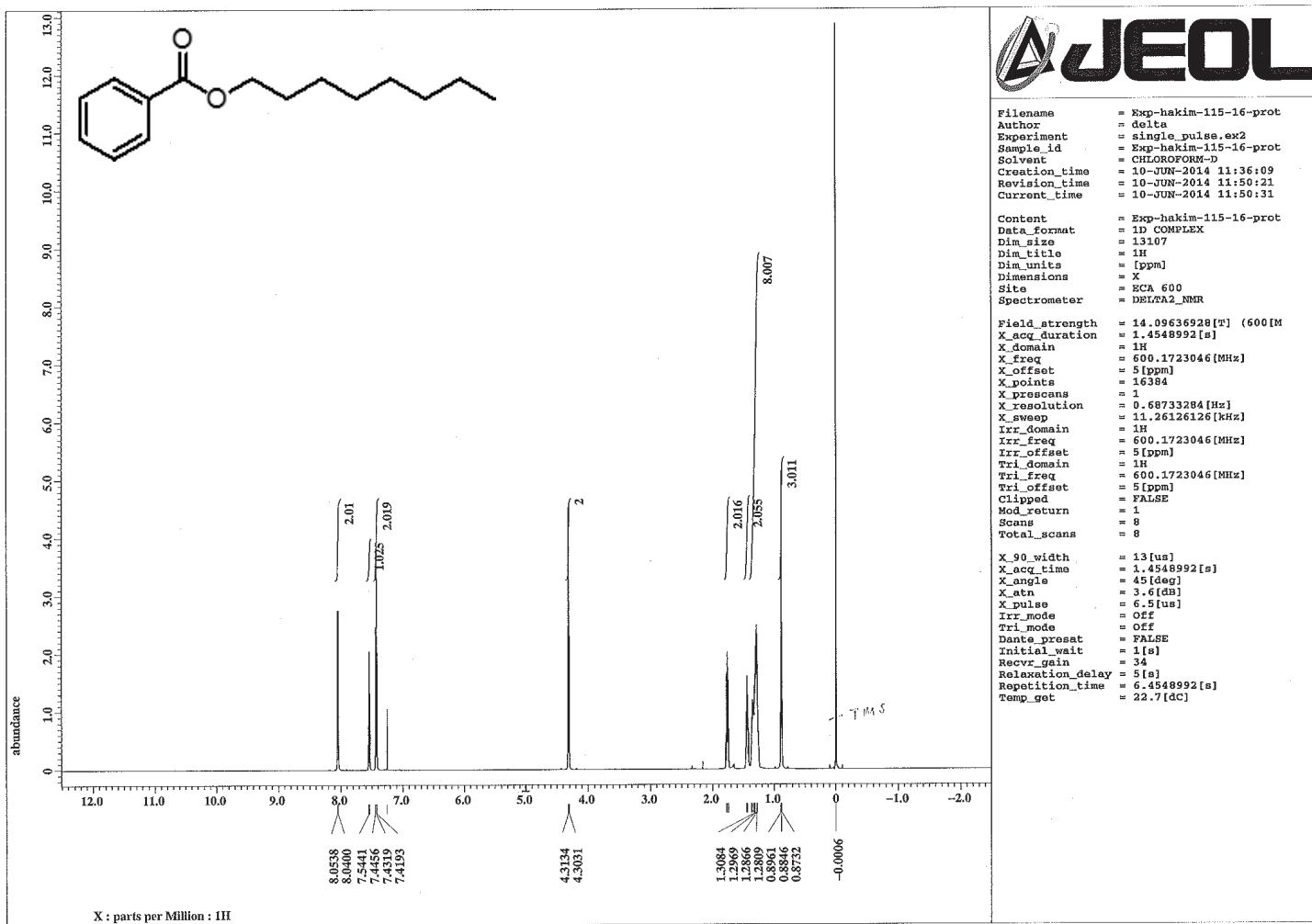


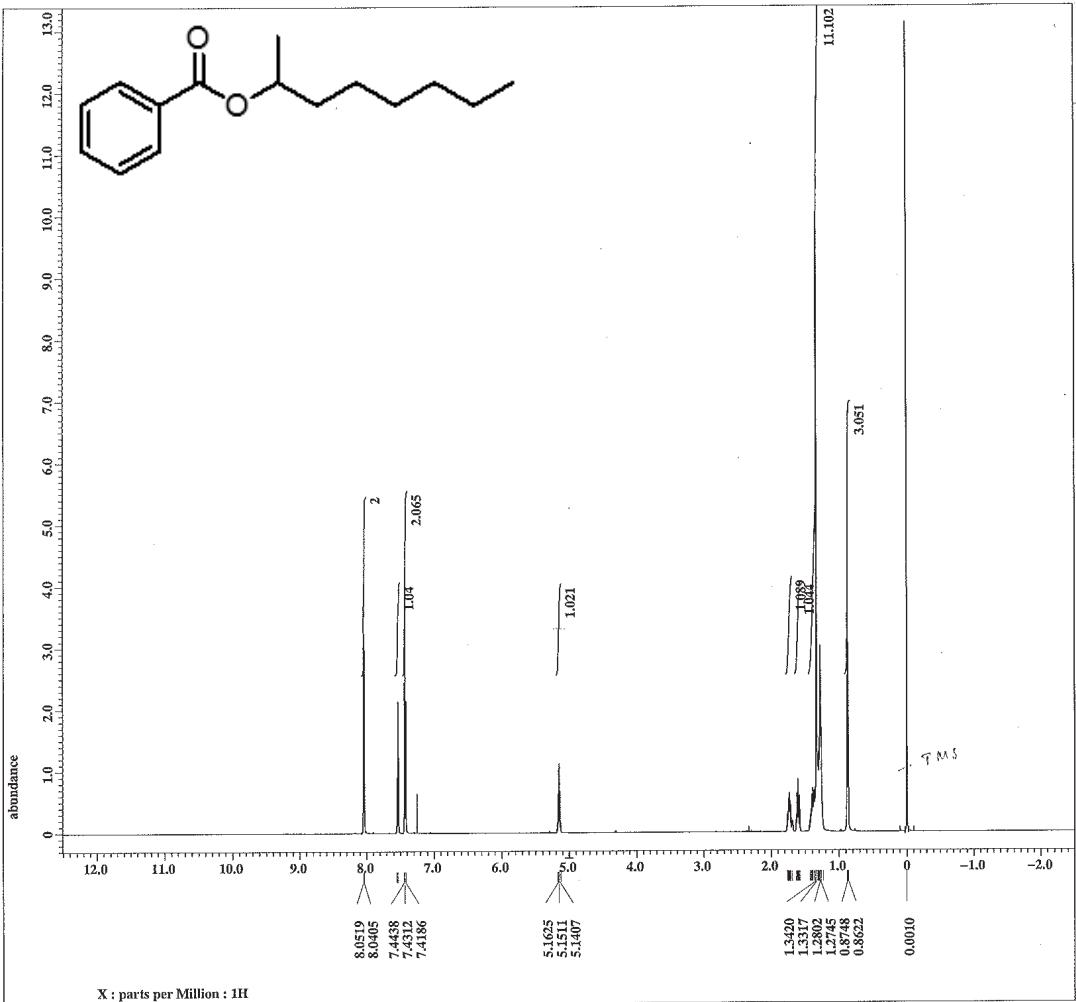
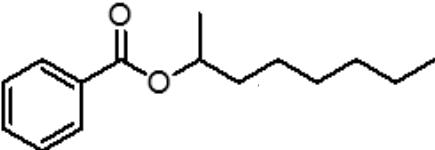






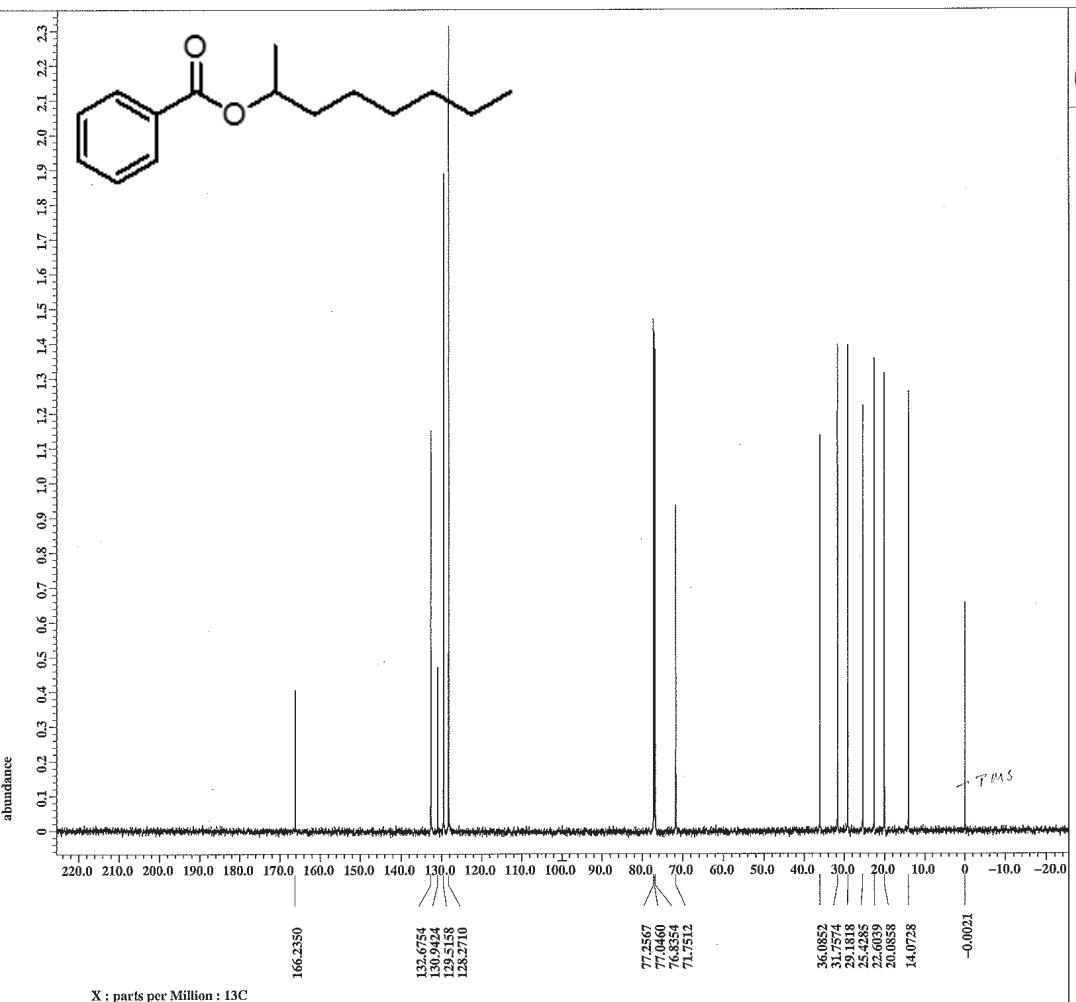






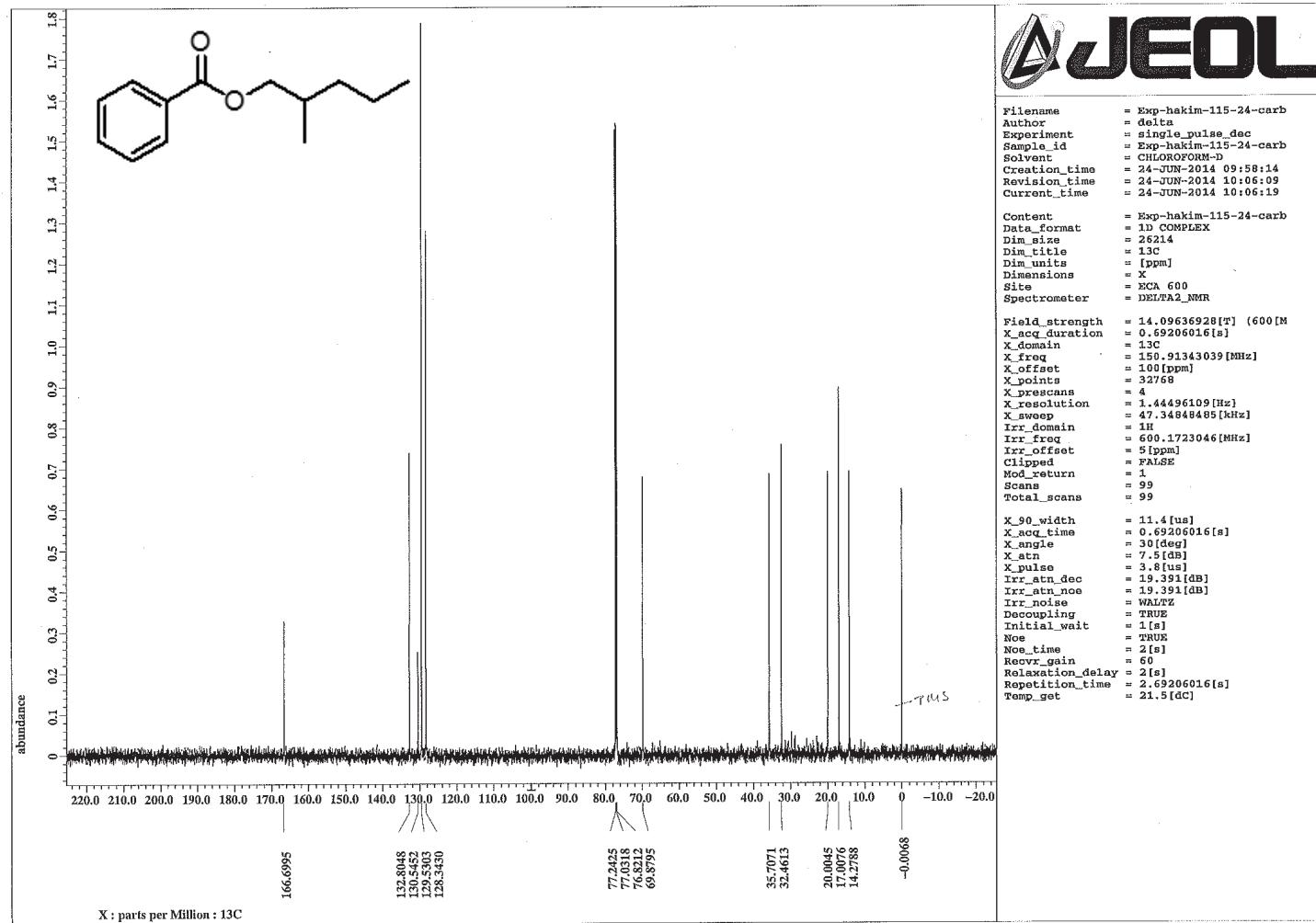
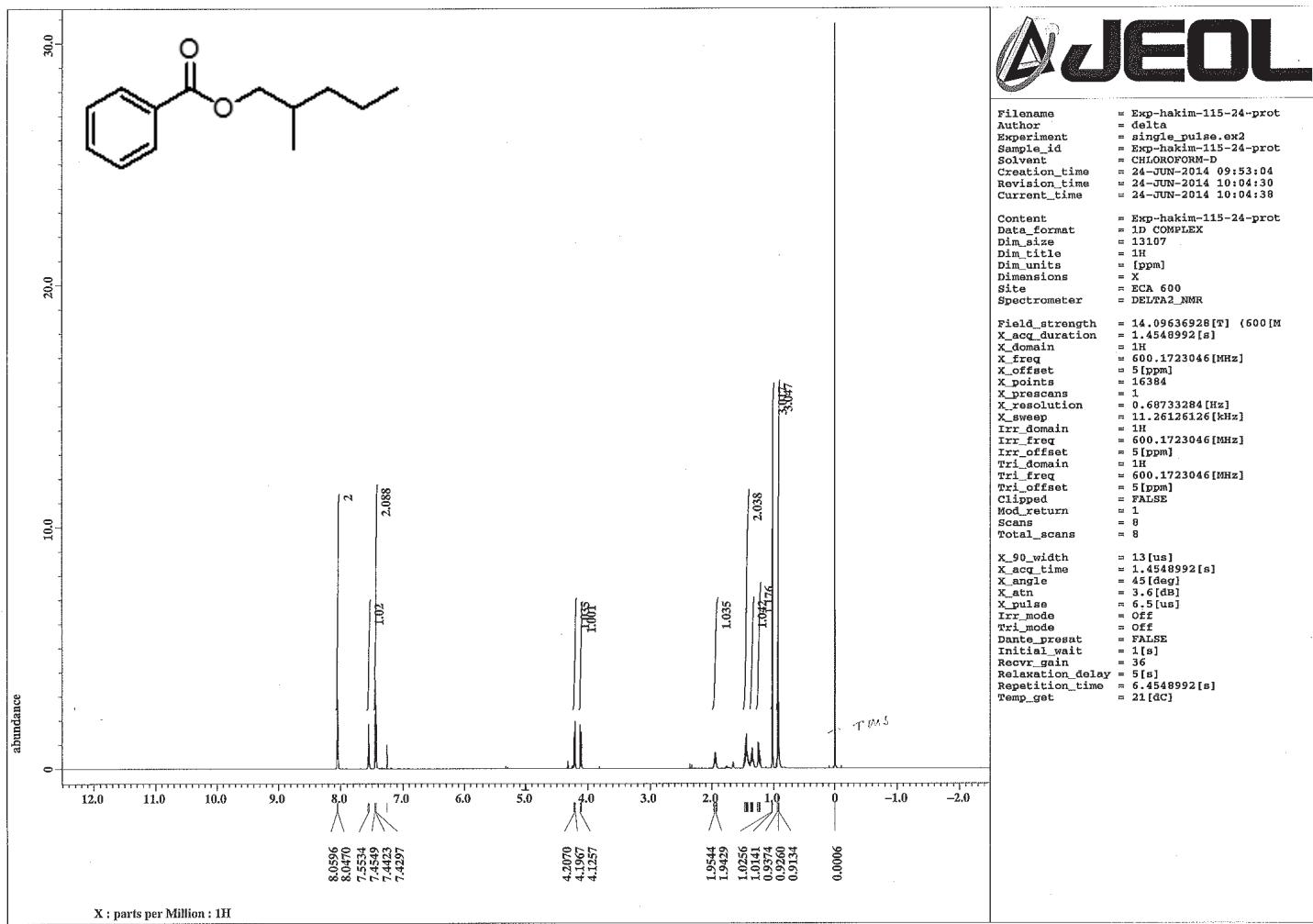
X : parts per Million : 1H

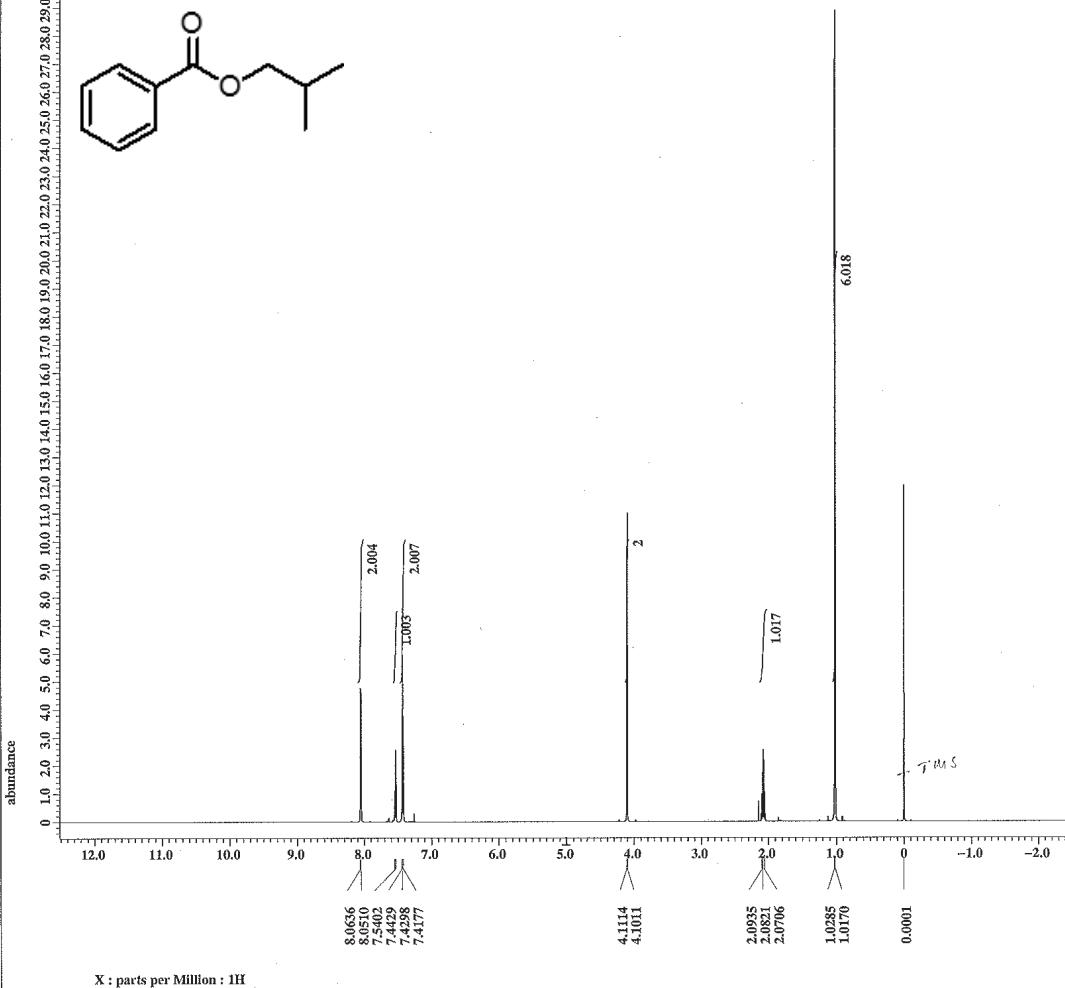
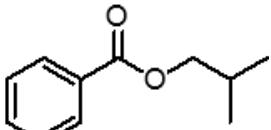
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X : parts per Million : 13C

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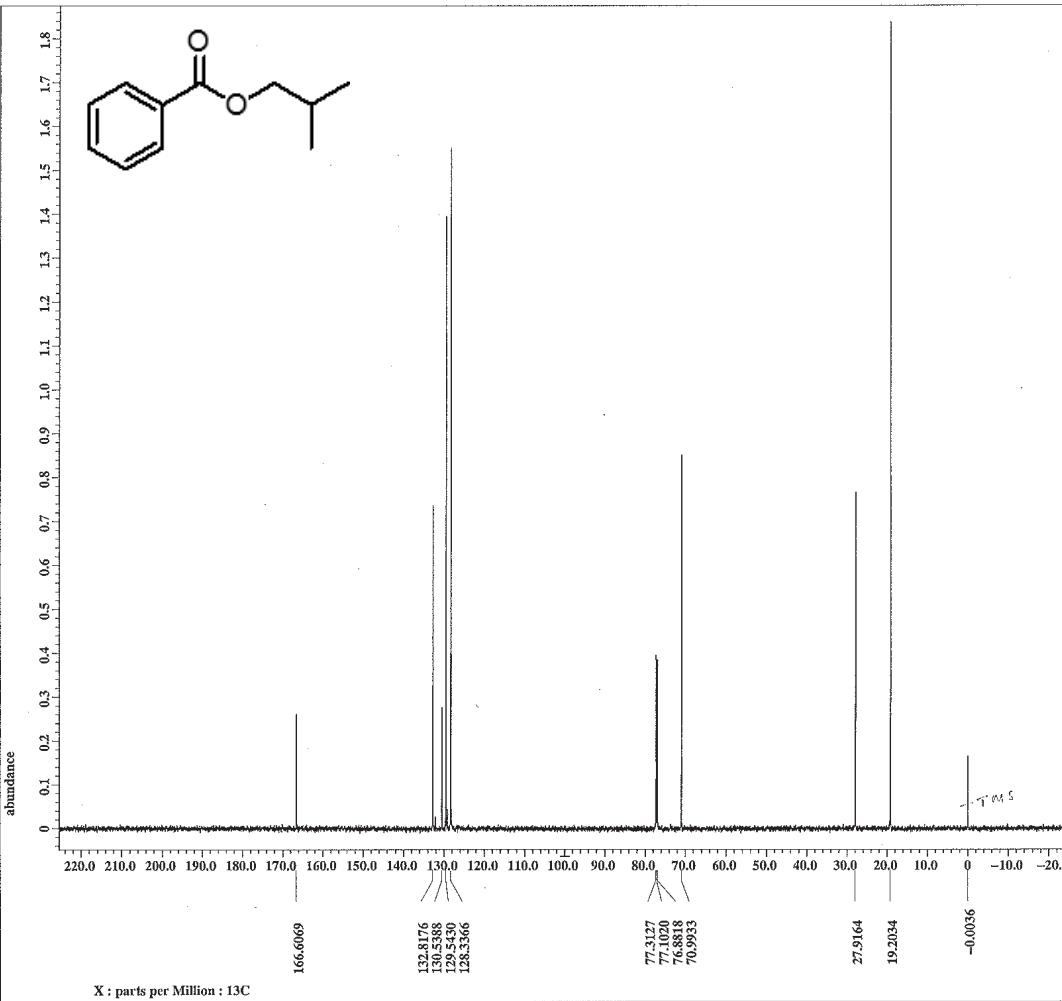
Filename = Exp-hakim-315-1-proto
Author = Delta
Experiment = single_pulse.ex2
Sample_id = Exp-hakim-315-1-proto
Solvent = CHLOROFORM-D
Creation_time = 17-JUN-2014 16:40:46
Revision_time = 17-JUN-2014 16:49:24
Current_time = 17-JUN-2014 16:49:33

Content = Exp-hakim-315-1-proto
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[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.5[us]
Irr_mode = QCP
Danto_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get = 21[dc]

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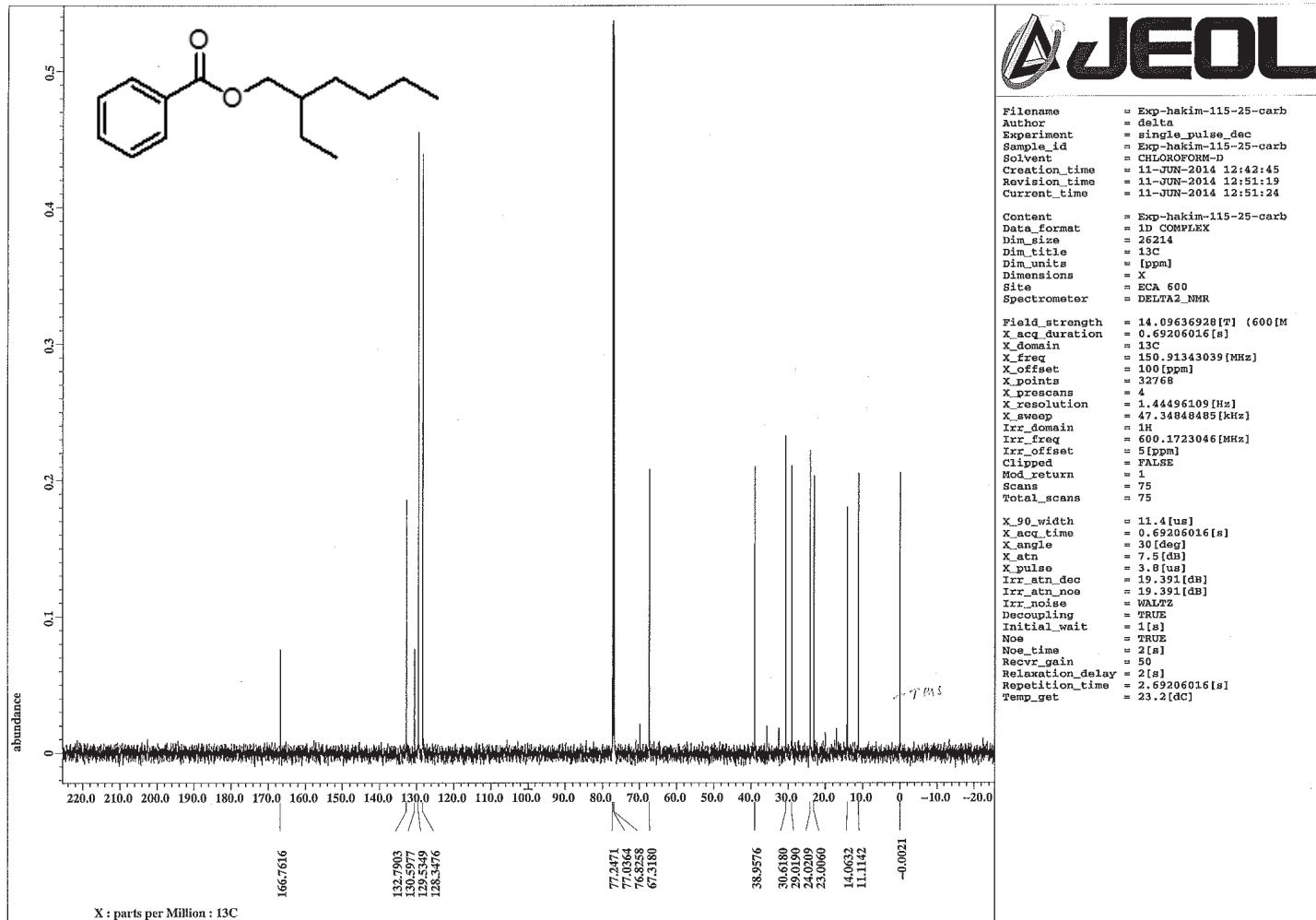
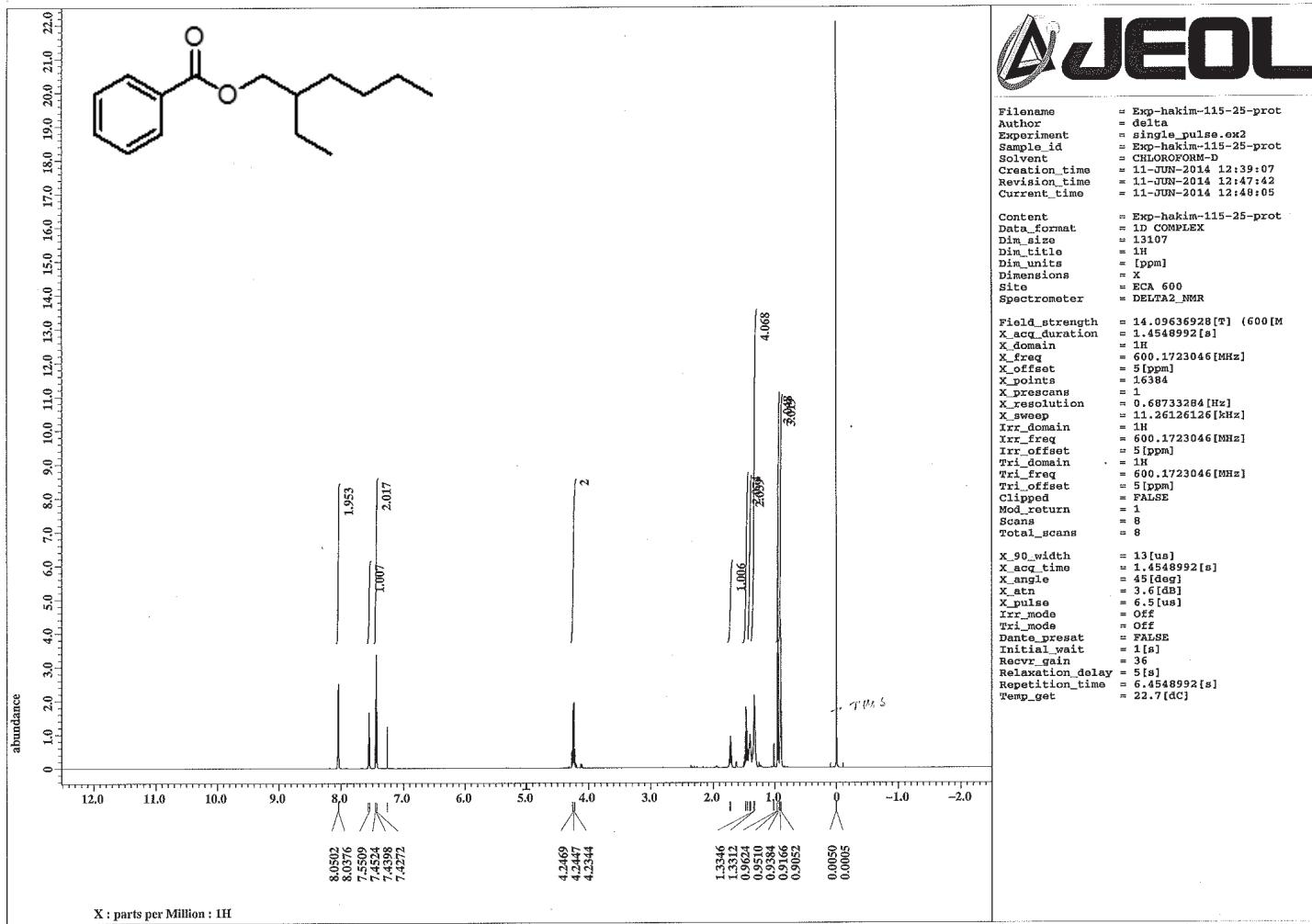
Filename = Exp-hakim-315-1-carbo
Author = delta
Experiment = single_pulse_dec
Sample_id = Exp-hakim-315-1-carbo
Solvent = CHLOROFORM-D
Creation_time = 17-JUN-2014 16:44:39
Revision_time = 17-JUN-2014 16:52:27
Current_time = 17-JUN-2014 16:52:36

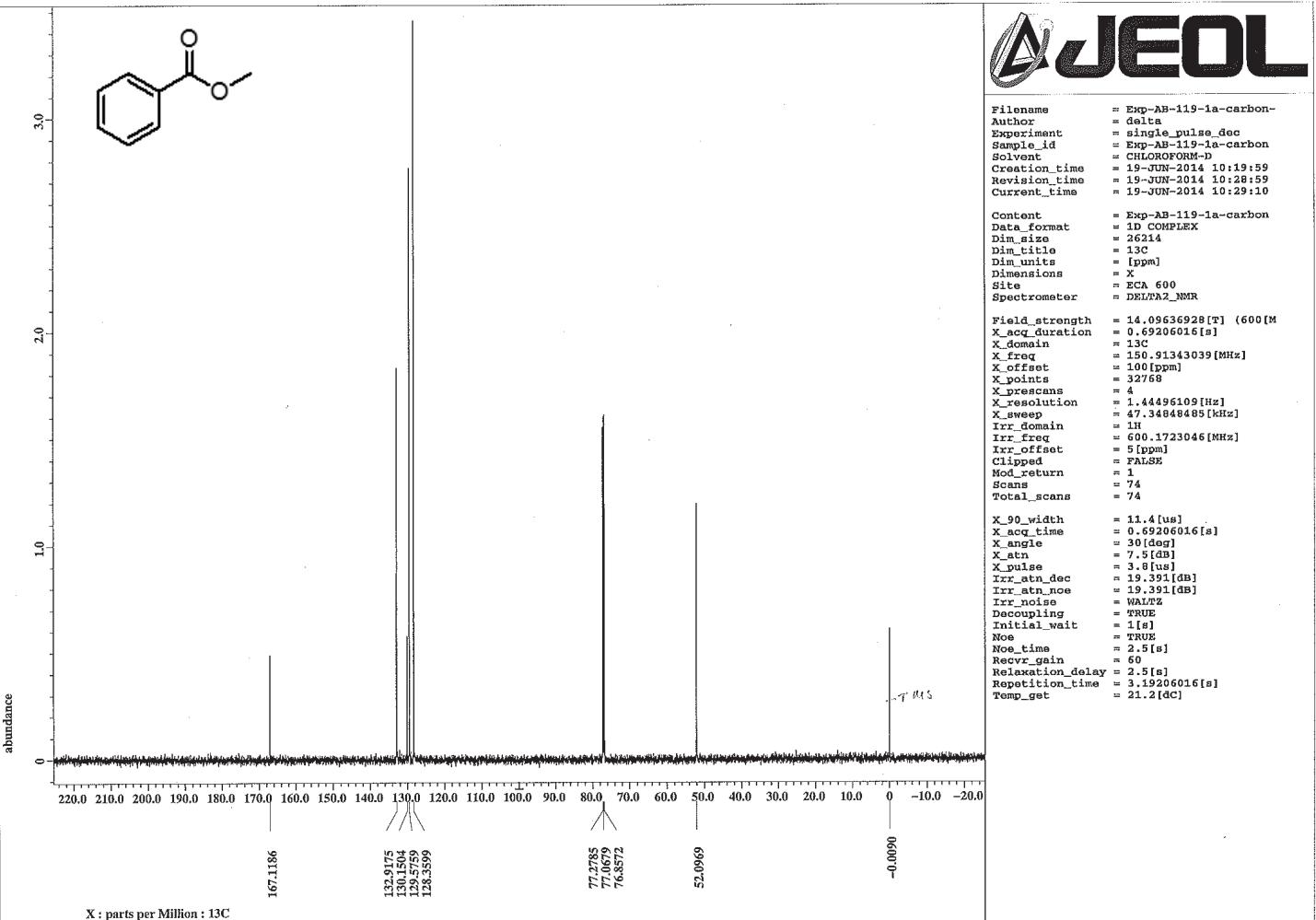
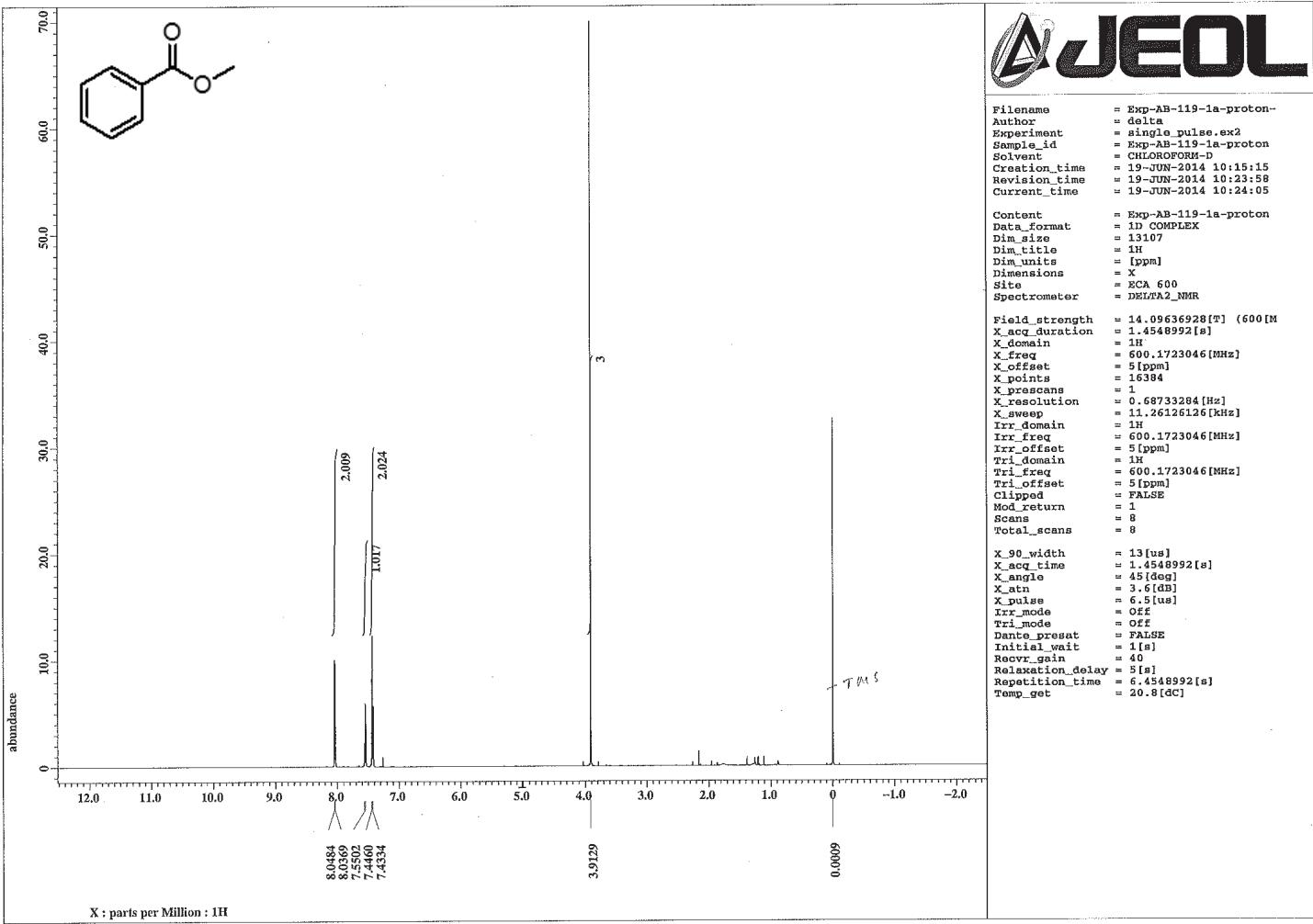
Content = Exp-hakim-315-1-carbo
Data_format = 1H COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DELTA2_NMR

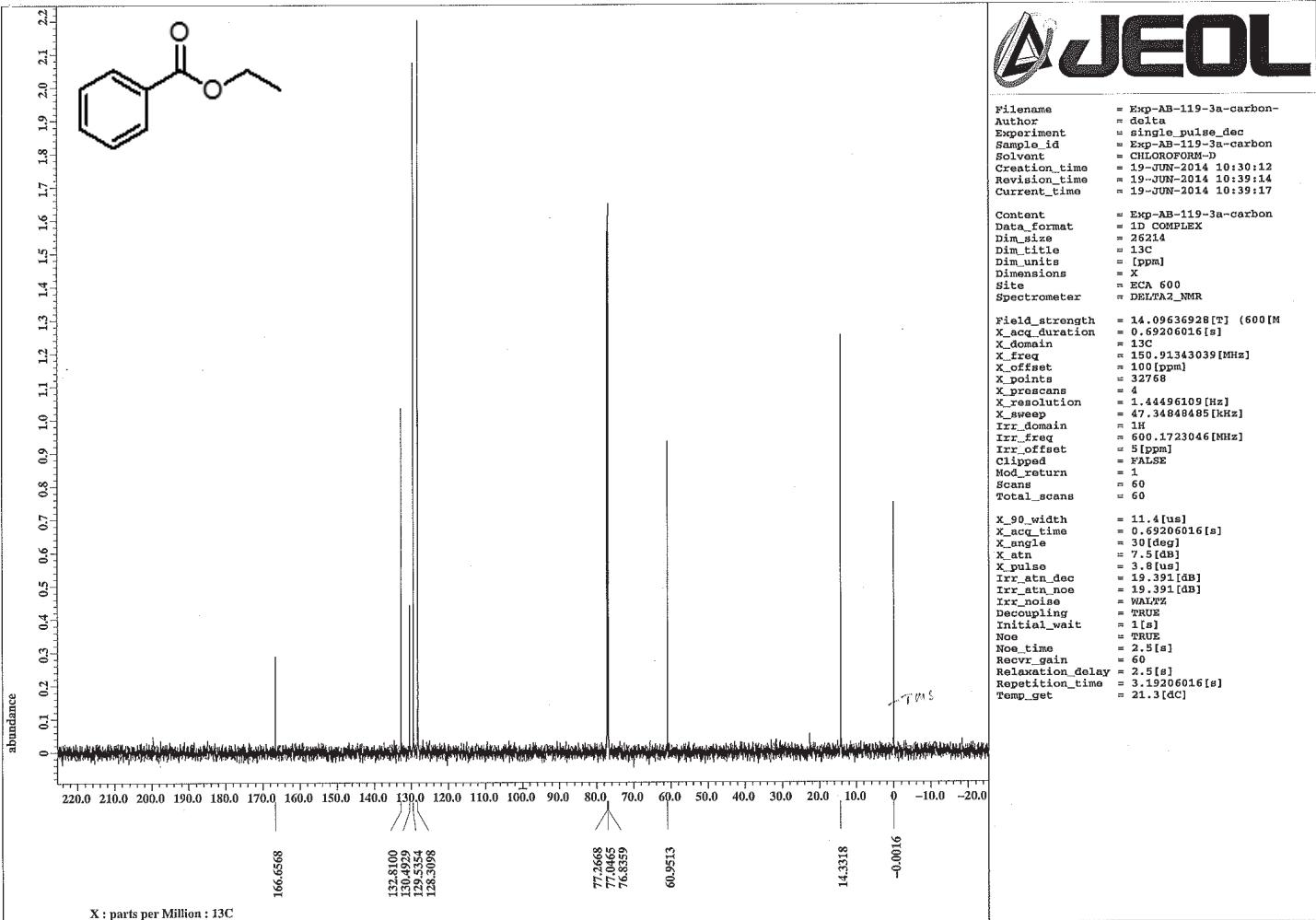
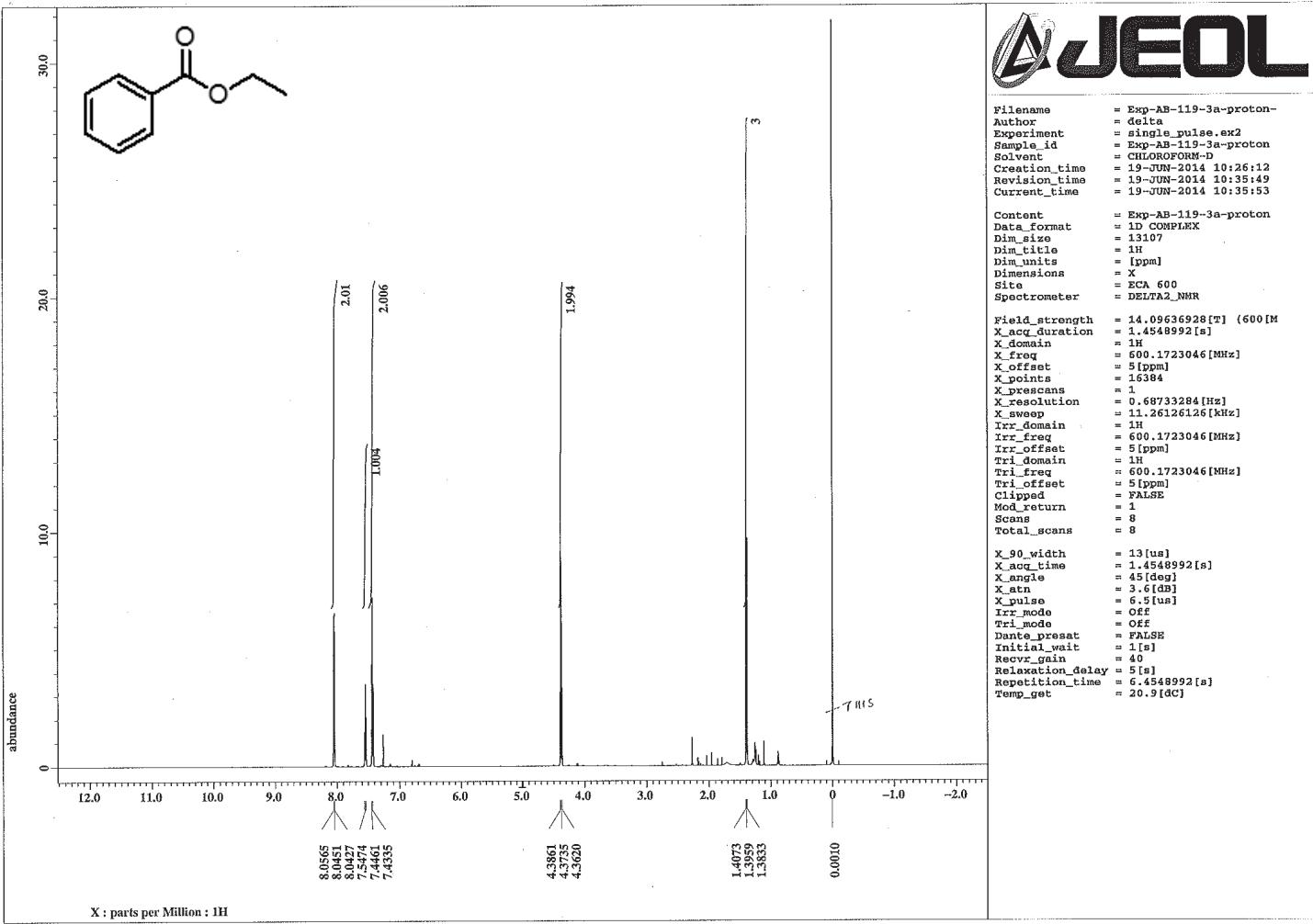
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 81
Total_scans = 81

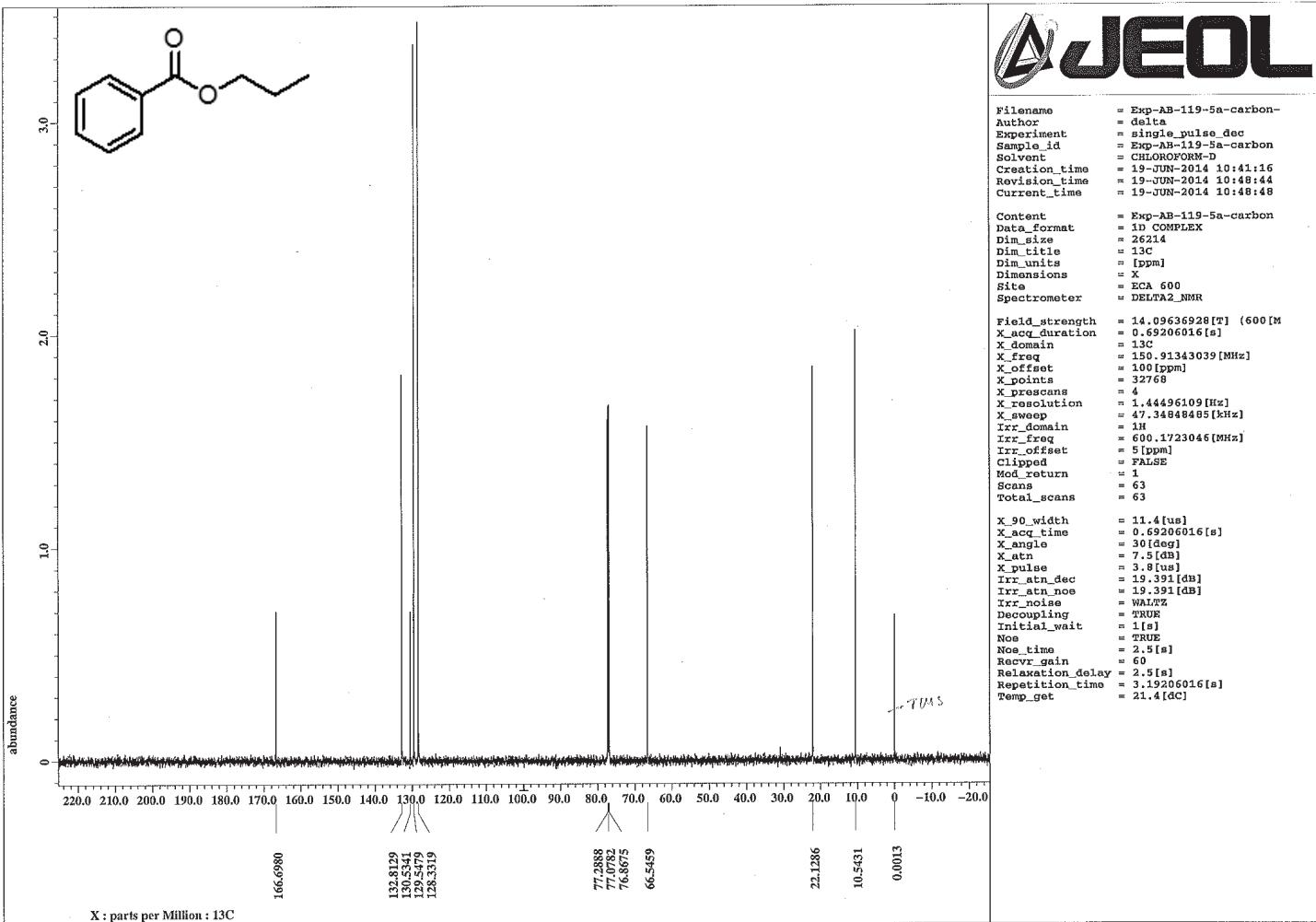
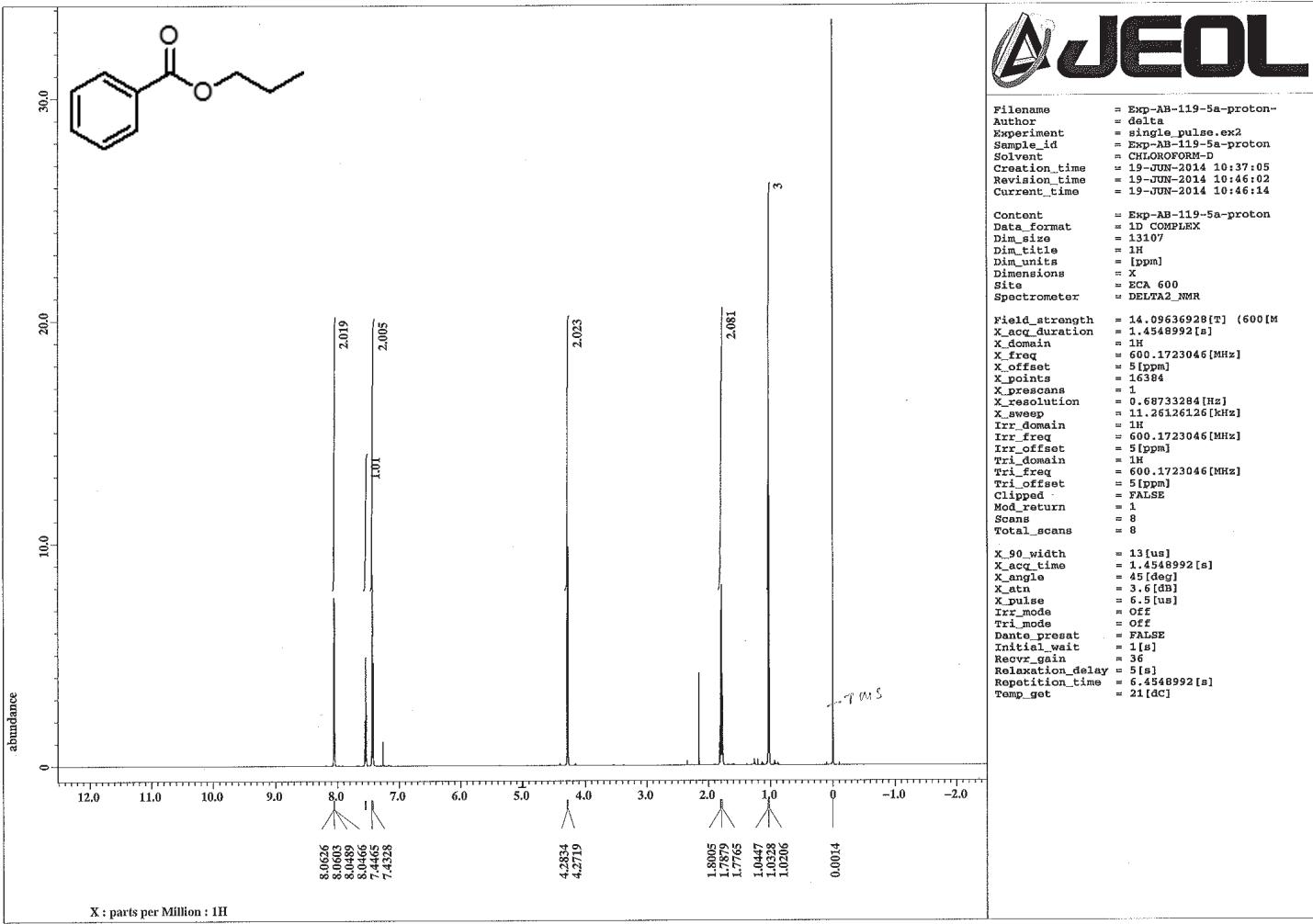
X_90_width = 11.4[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 3.8[us]
Irr_atn_dec = 19.391[dB]
Irr_atn_noe = 19.391[dB]
Irr_noise = WALZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get = 21.7[dc]

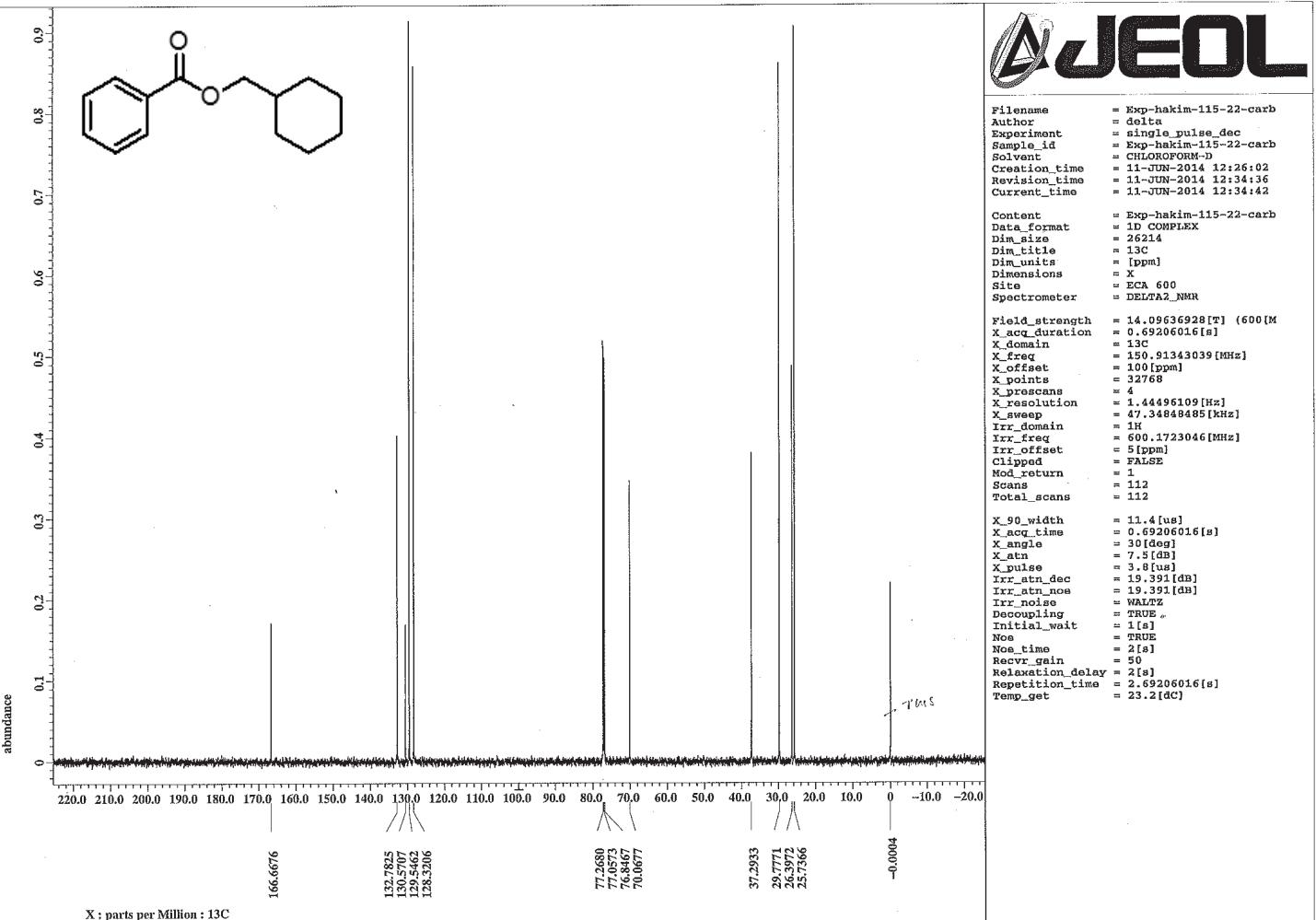
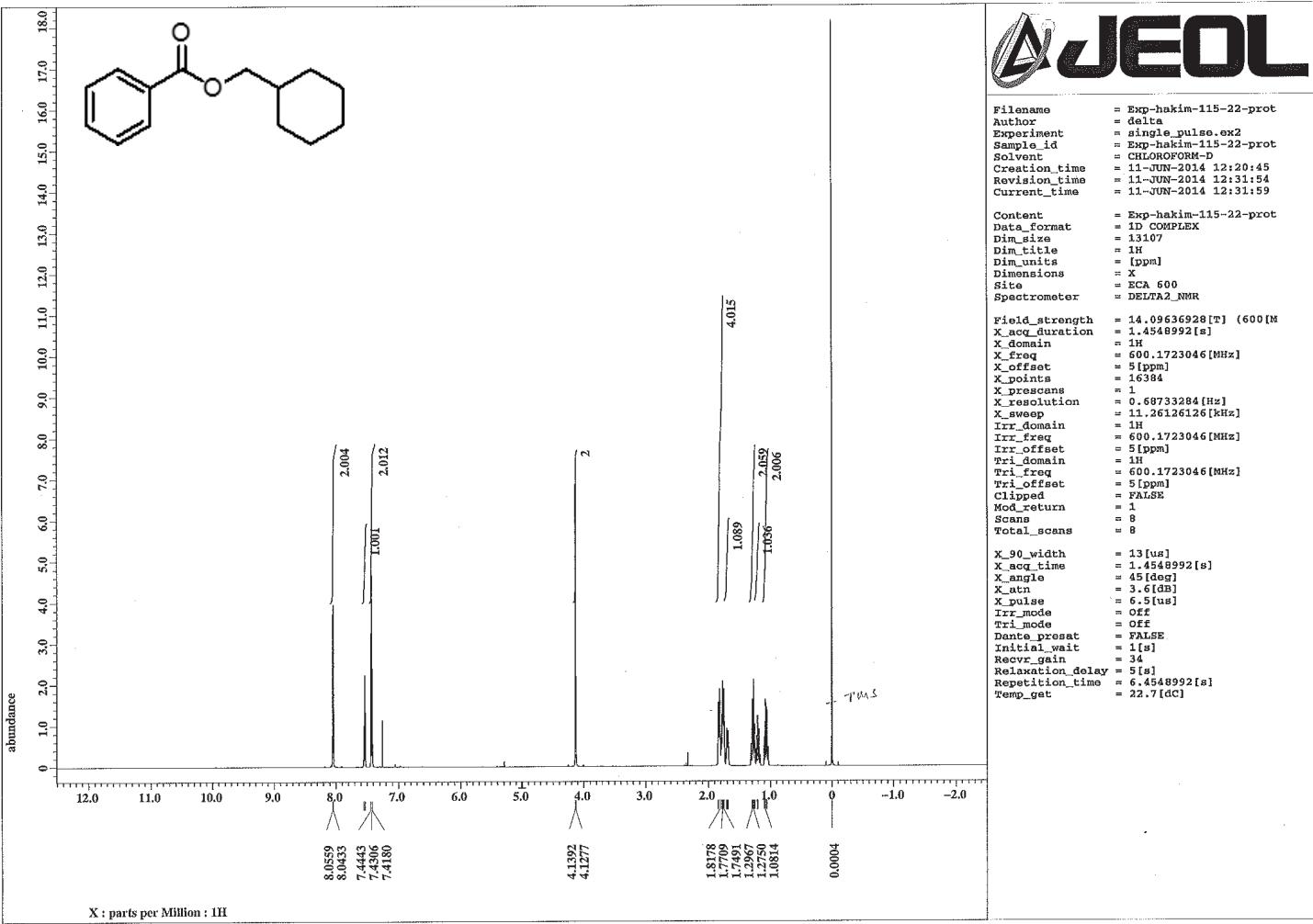
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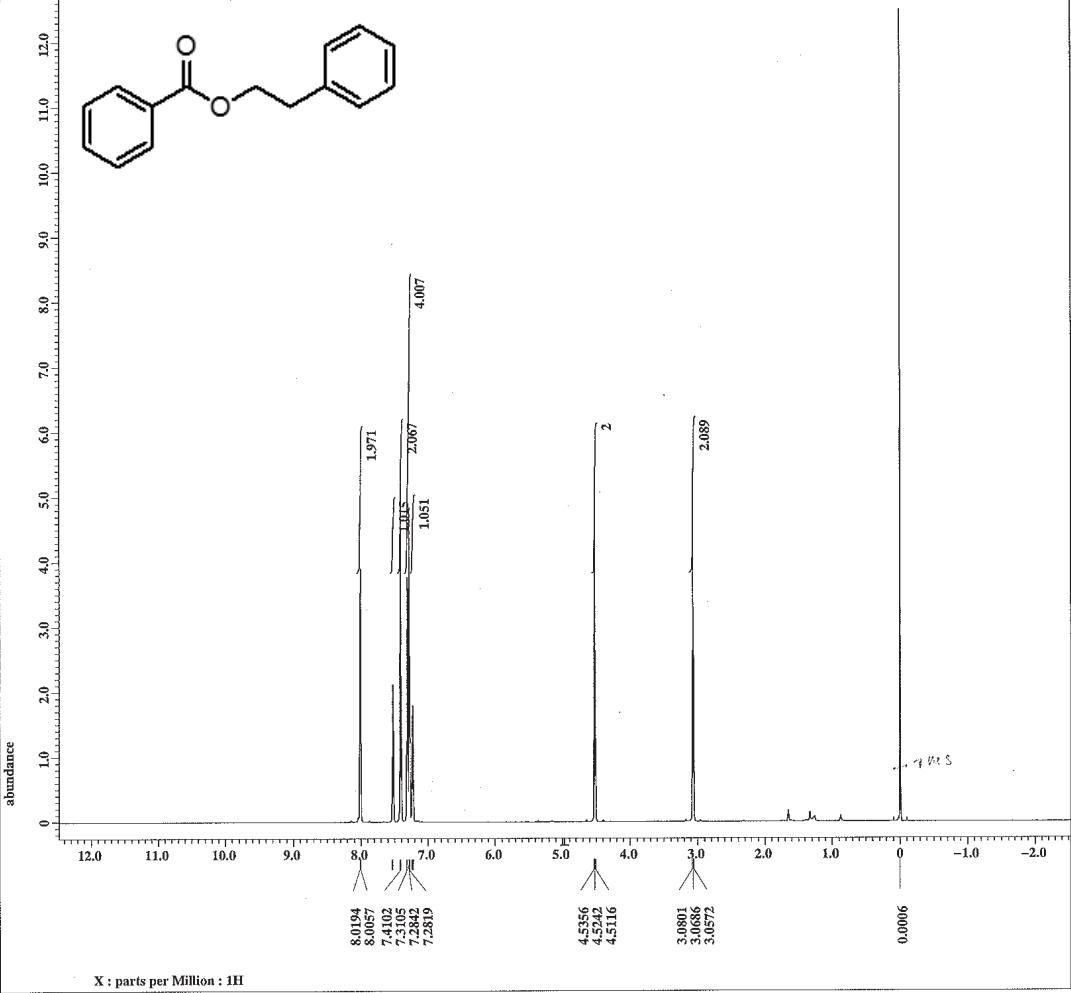
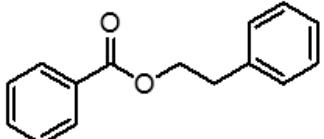












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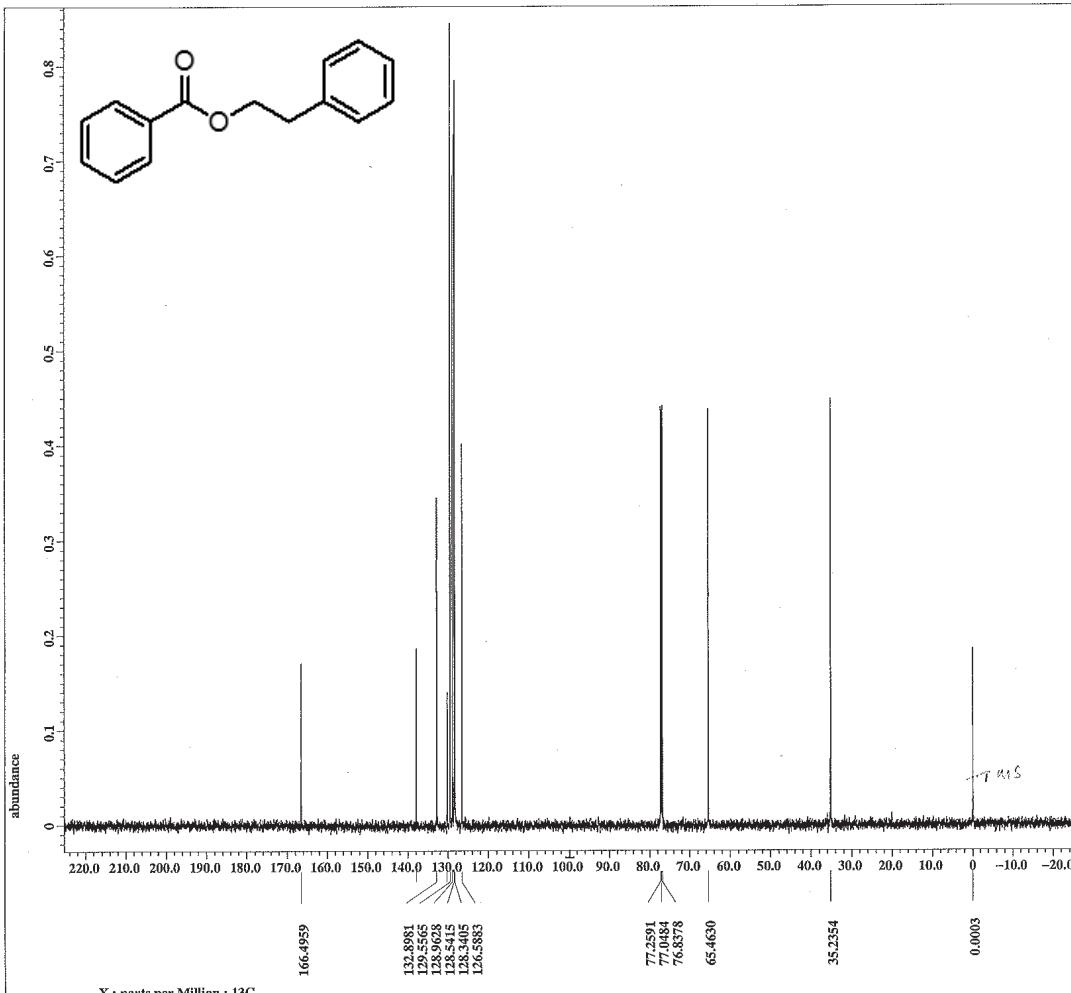
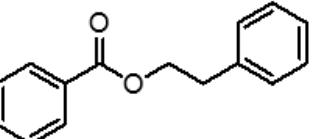
Filename = Exp-hakim-115-18-prot
Author = dcl1
Experiment = single_pulse.ex2
Sample_id = Exp-hakim-115-18-prot
Solvent = CHLOROFORM-D
Creation_time = 11-JUN-2014 12:03:59
Revision_time = 11-JUN-2014 12:13:39
Current_time = 11-JUN-2014 12:13:45

Content = Exp-hakim-115-18-prot
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_pulse = 16384
X_prescans = 1
X_resolution = 0.69733284[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[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atr = 3.6[dB]
X_pulse = 6.5[us]
Irr_mode = OFF
Tri_mode = OFF
Densitogram = FALSE
Initial_wait = 0[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get = 22.8[dC]

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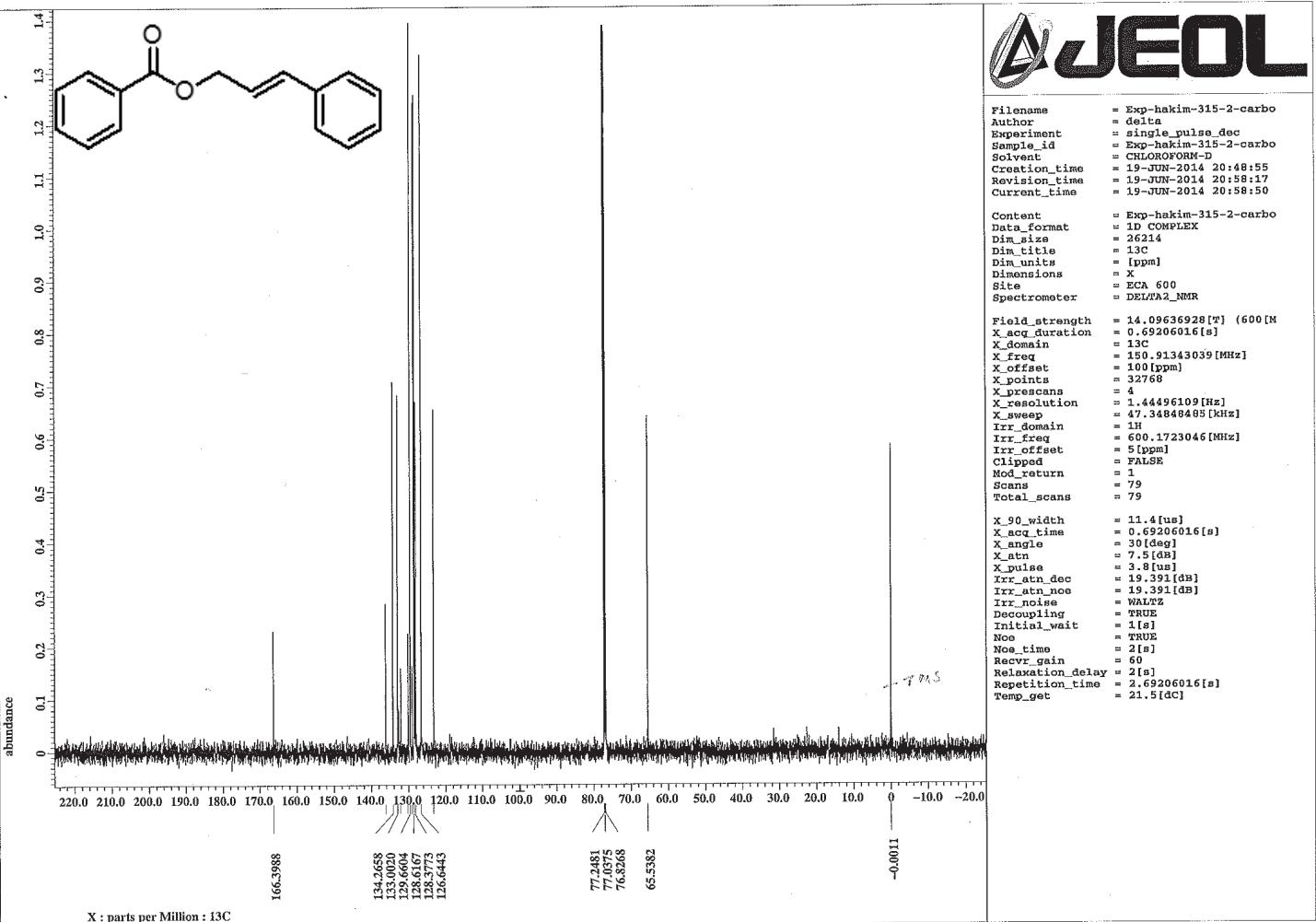
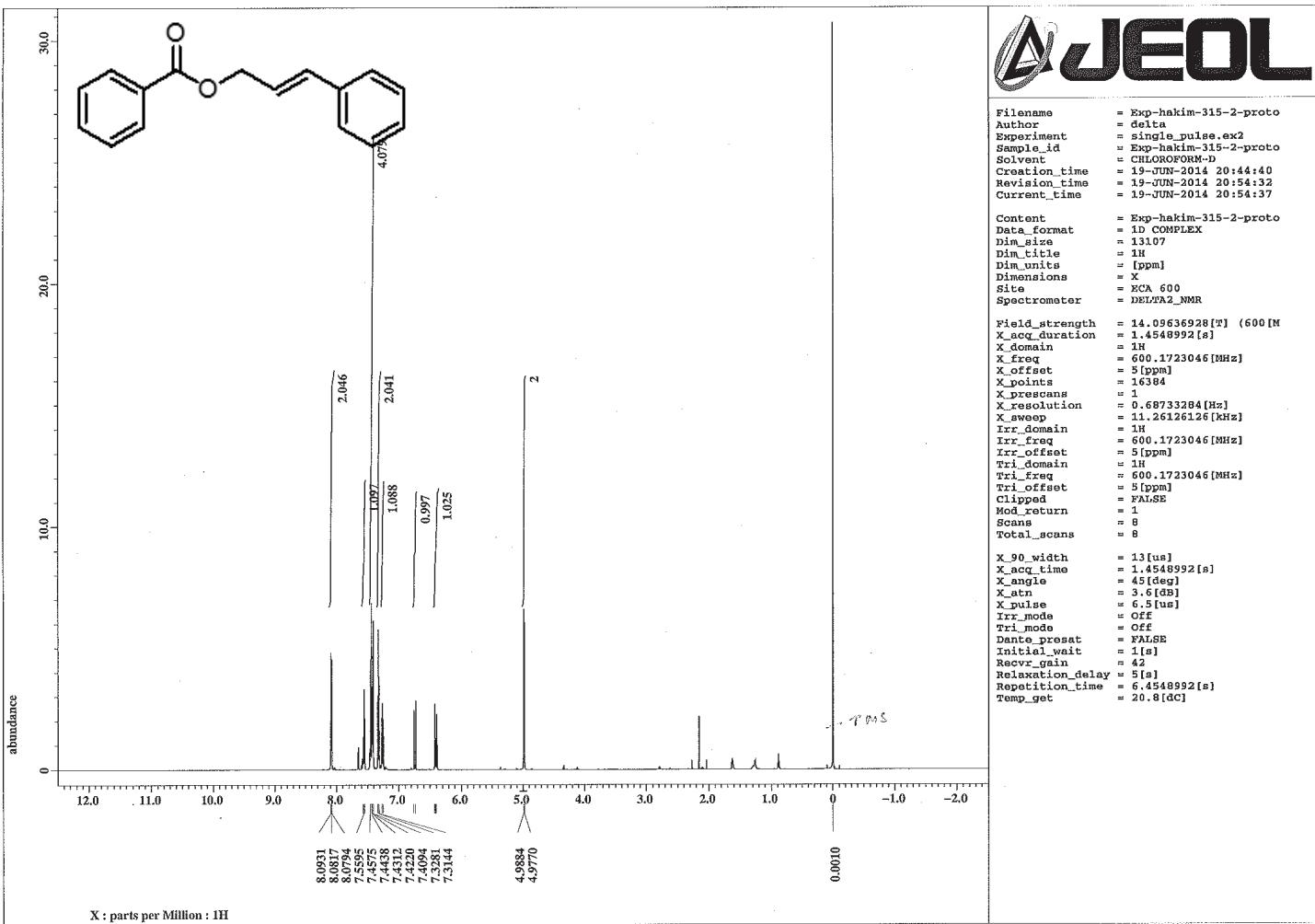
Filename = Exp-hakim-115-18-carb
Author = dcl1
Experiment = single_pulse_dec
Sample_id = Exp-hakim-115-18-carb
Solvent = CHLOROFORM-D
Creation_time = 11-JUN-2014 12:02:15
Revision_time = 11-JUN-2014 12:09:35
Current_time = 11-JUN-2014 12:09:39

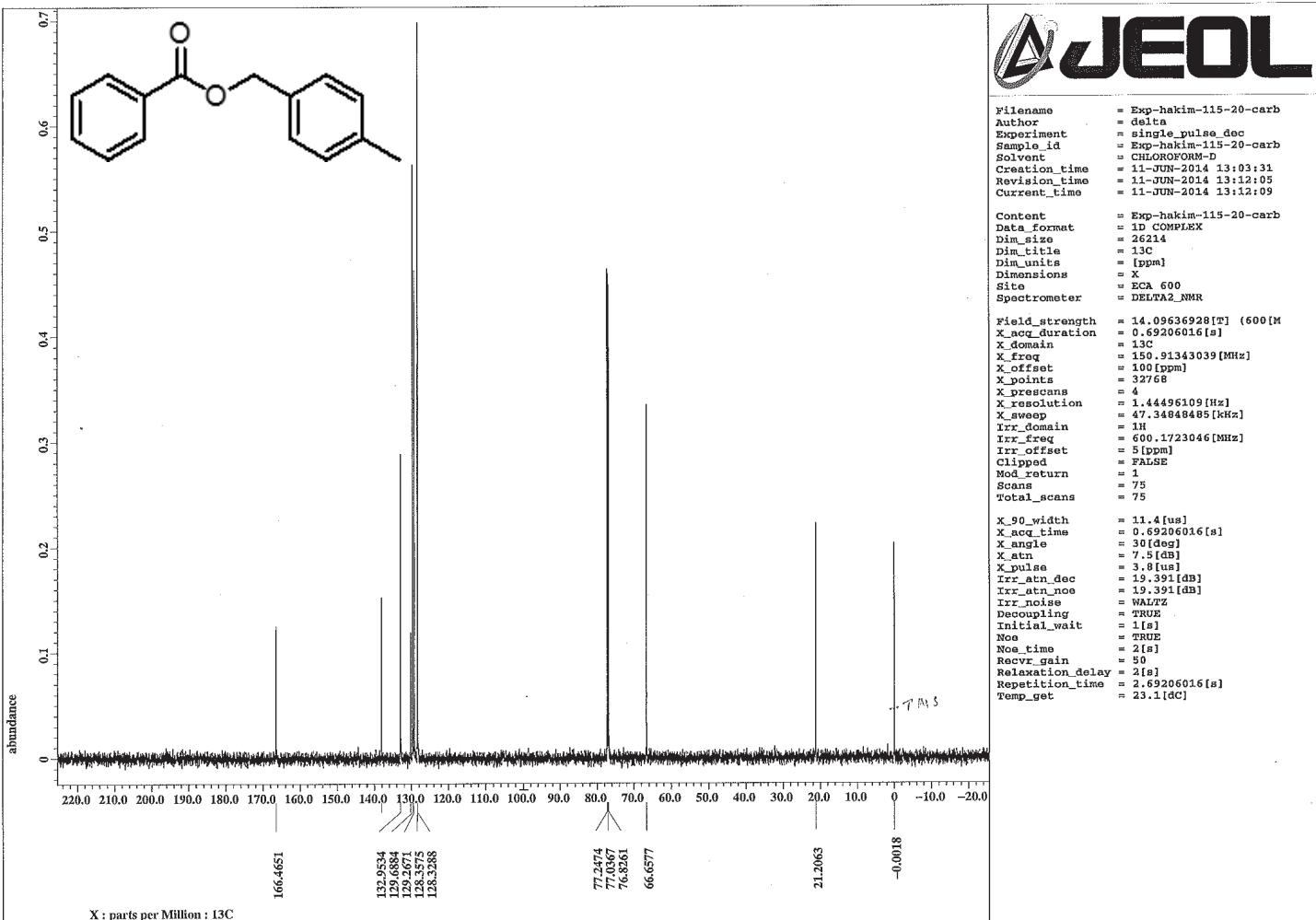
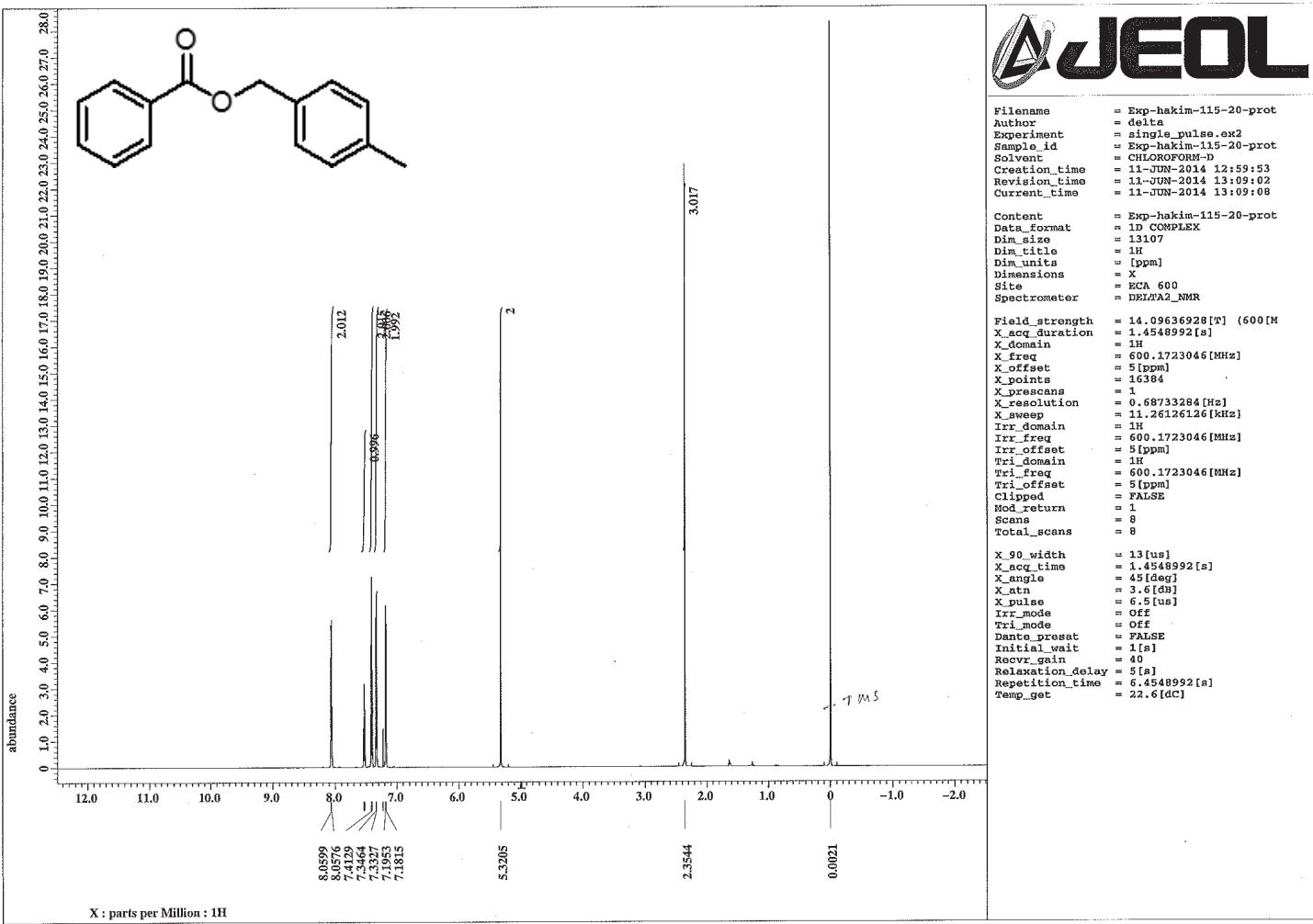
Content = Exp-hakim-115-18-carb
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DELTA2_NMR

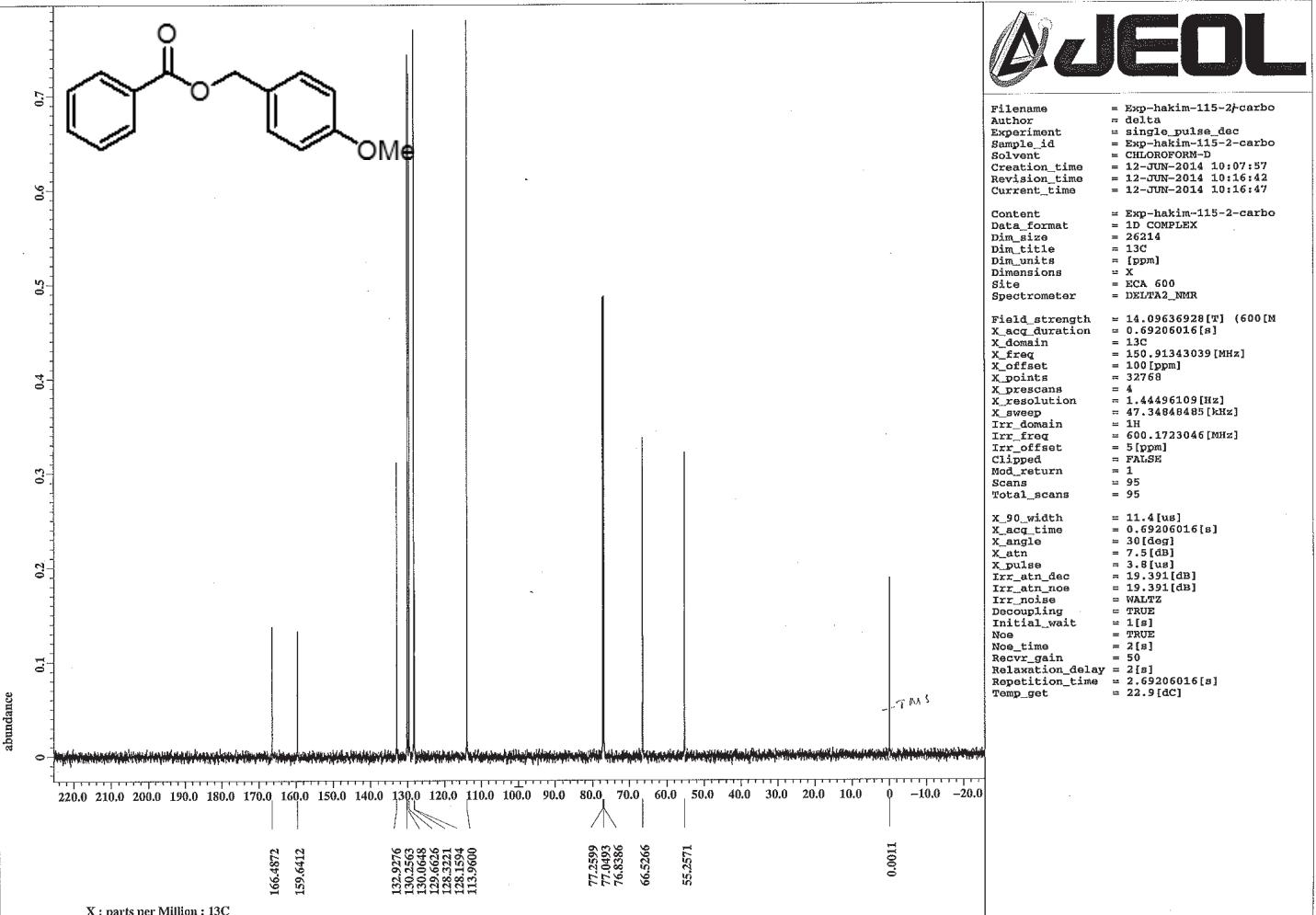
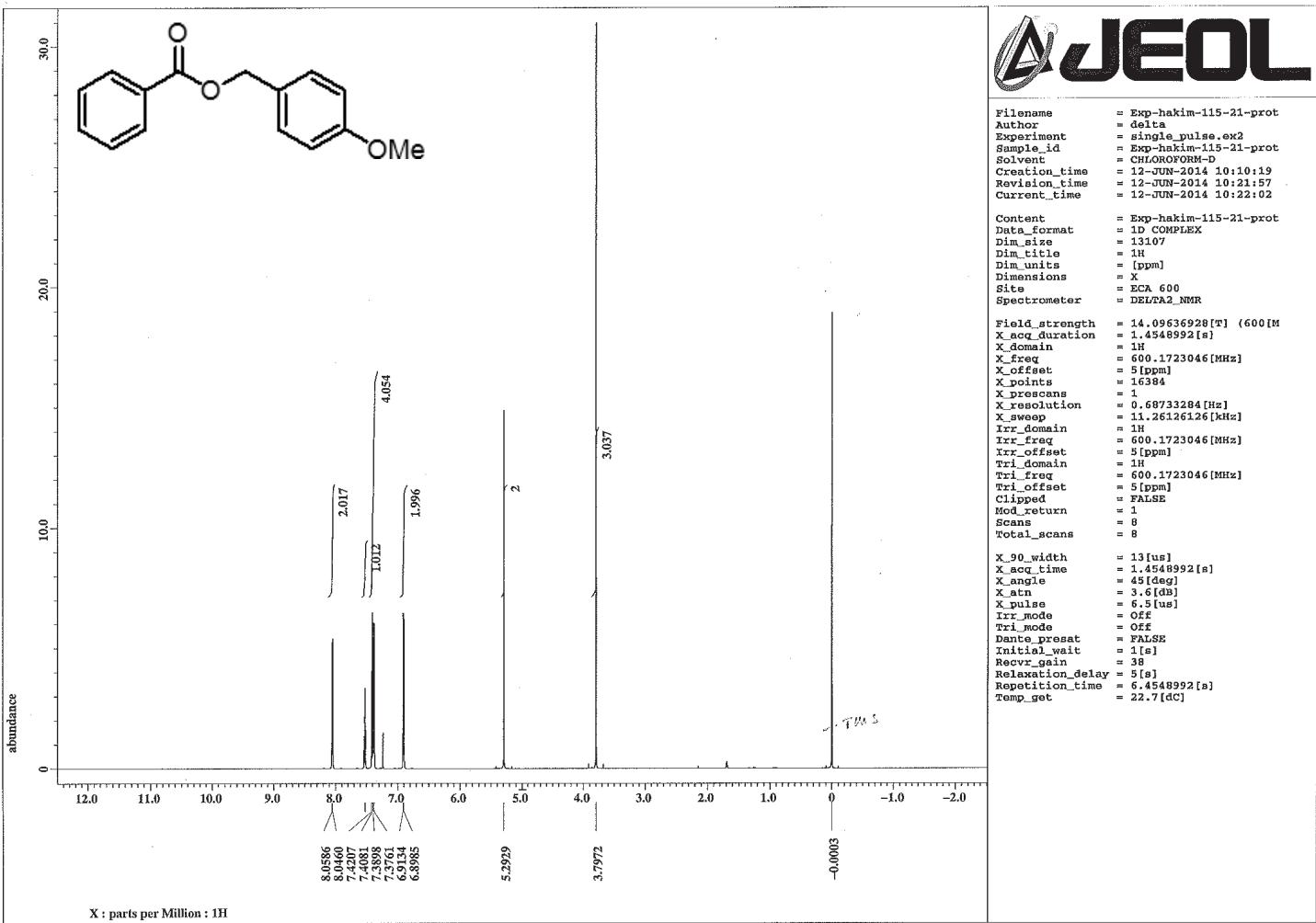
Field_strength = 14.09636928[T] (600[N
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[NHz]
X_offset = 100[ppm]
X_pulses = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34648485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 95
Total_scans = 95

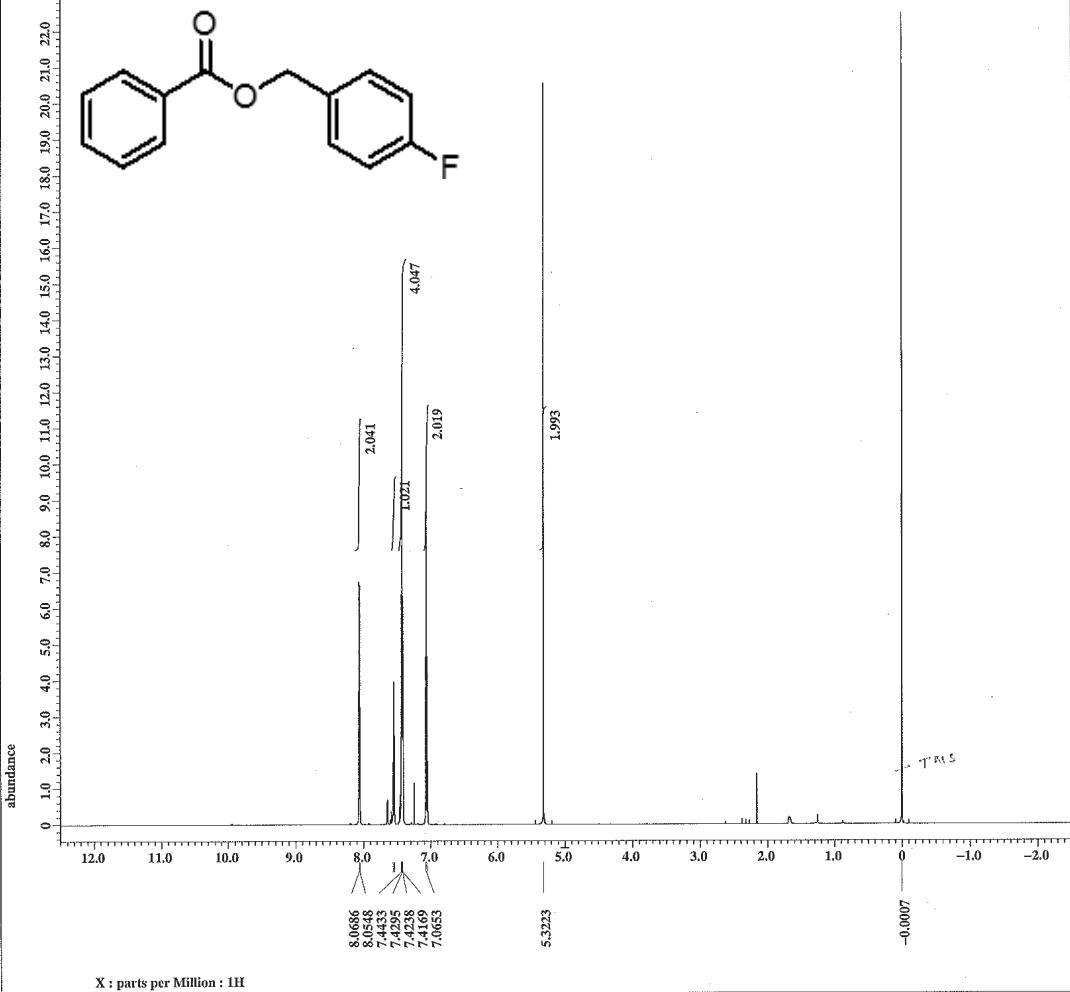
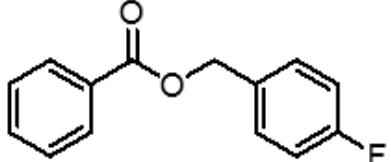
X_90_width = 11.4[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atr = 7.5[dB]
X_pulse = 3.8[us]
Irr_atr_dec = 19.391[dB]
Irr_atr_noe = 19.391[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe_time = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get = 23.1[dC]

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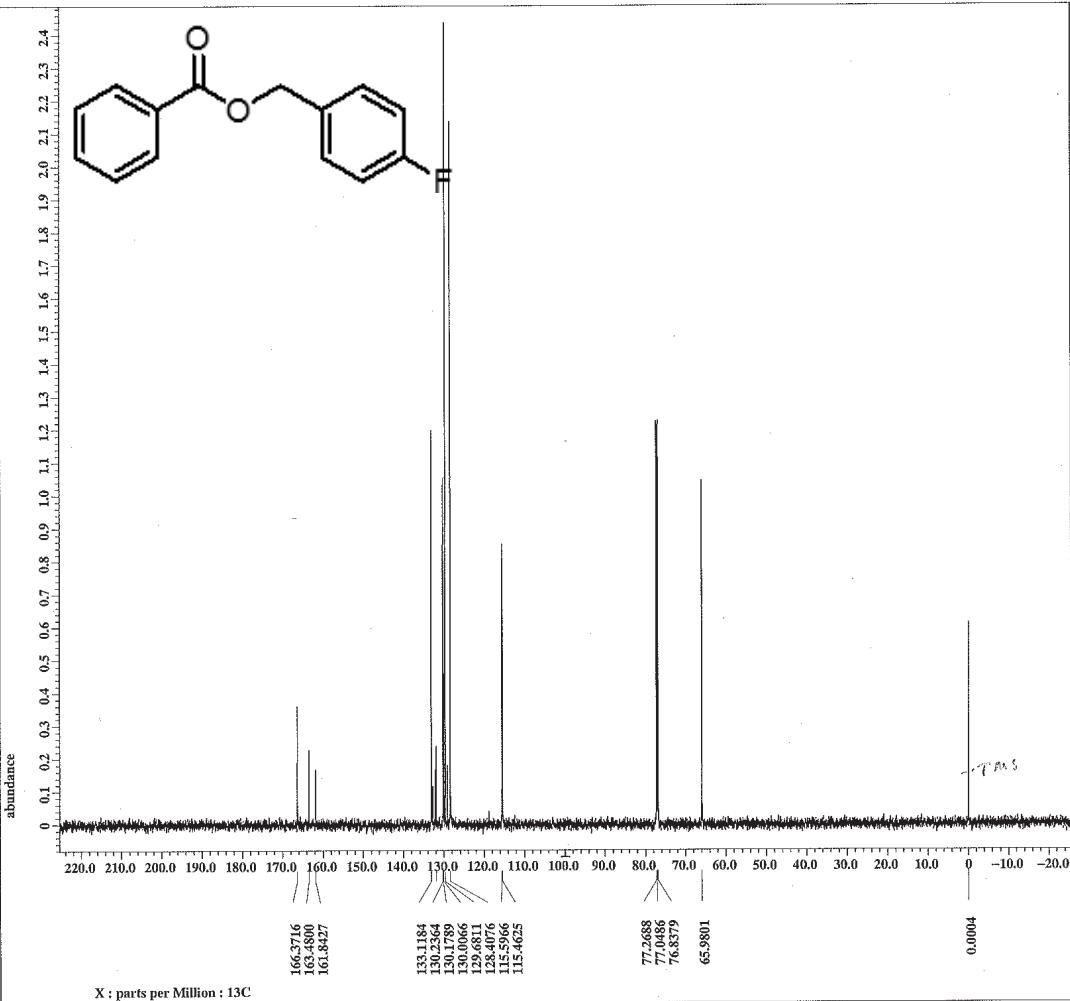
filename = Exp-AB-114-7-proton-6
author = delta
Experiment = single_pulse_ex2
sample_id = Exp-AB-114-7-proton
Solvent = CHLOROFORM-D
Creation_time = 19-JUN-2014 22:18:42
Revision_time = 12-JUL-2014 11:32:55
Current_time = 12-JUL-2014 11:33:03

Content = EXP-AB-114-7-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 = IH
X_offset = 600.1723046[NHz]
X_points = 51[ppm]
X_prescans = 16384
X_resolution = 0.68733284[Hz]
X_sweep = 11.26126126[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[NHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[NHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 13[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.5[us]
Irr_atn = 0.5[dB]
Tri_mode = OFF
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get = 21.1[dc]

```



JEOL

```

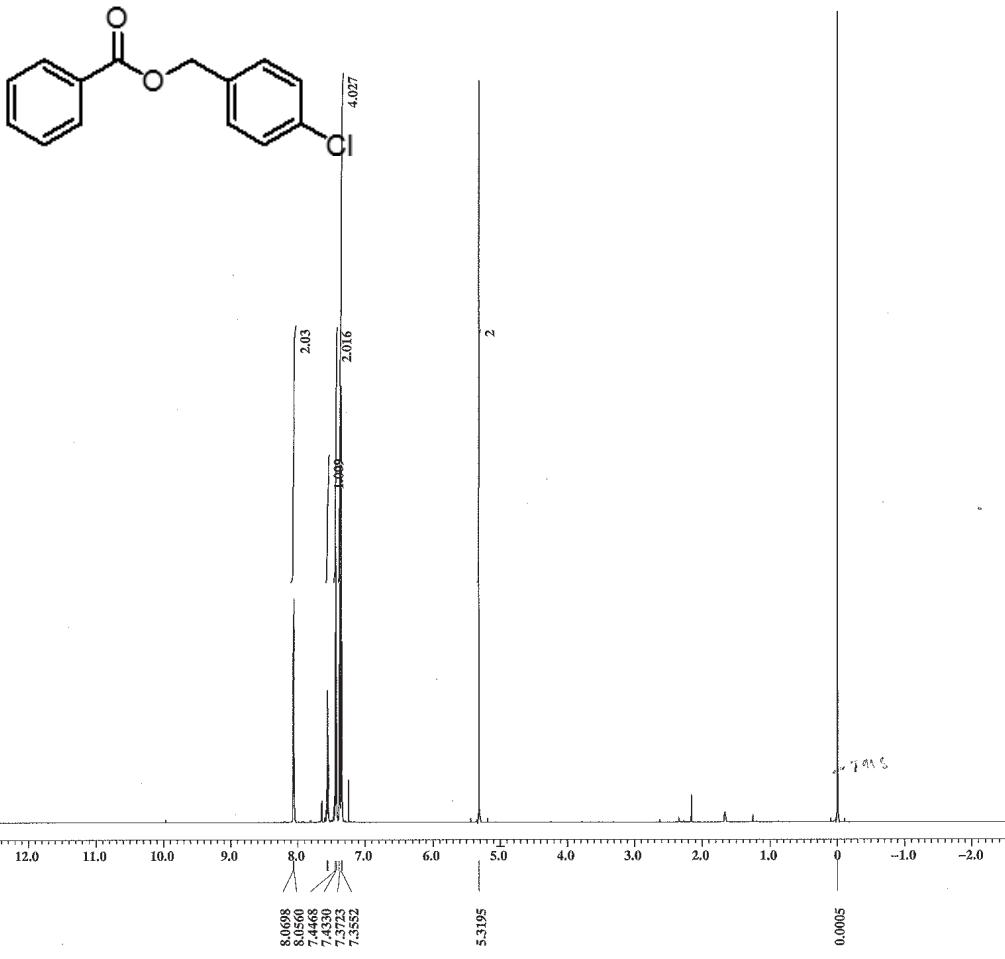
filename = Exp-AB-114-7-carbon-4
author = delta
Experiment = single_pulse_dec
sample_id = Exp-AB-114-7-carbon
Solvent = CHLOROFORM-D
Creation_time = 19-JUN-2014 22:24:21
Revision_time = 19-JUN-2014 22:34:41
Current_time = 19-JUN-2014 22:37:12

Content = EXP-AB-114-7-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_offset = 150.91343039[NHz]
X_points = 100[ppm]
X_prescans = 32768
X_resolution = 4[ppm]
X_sweep = 14.4496109[Hz]
Irr_domain = 1H
Irr_freq = 600.1723046[NHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 110
Total_scans = 110

X_90_width = 11.4[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 3.8[us]
Irr_atn_dec = 19.391[dB]
Irr_atn_noce = 19.391[dB]
Irr_noce = MMWZ
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]

```



JEOL

```

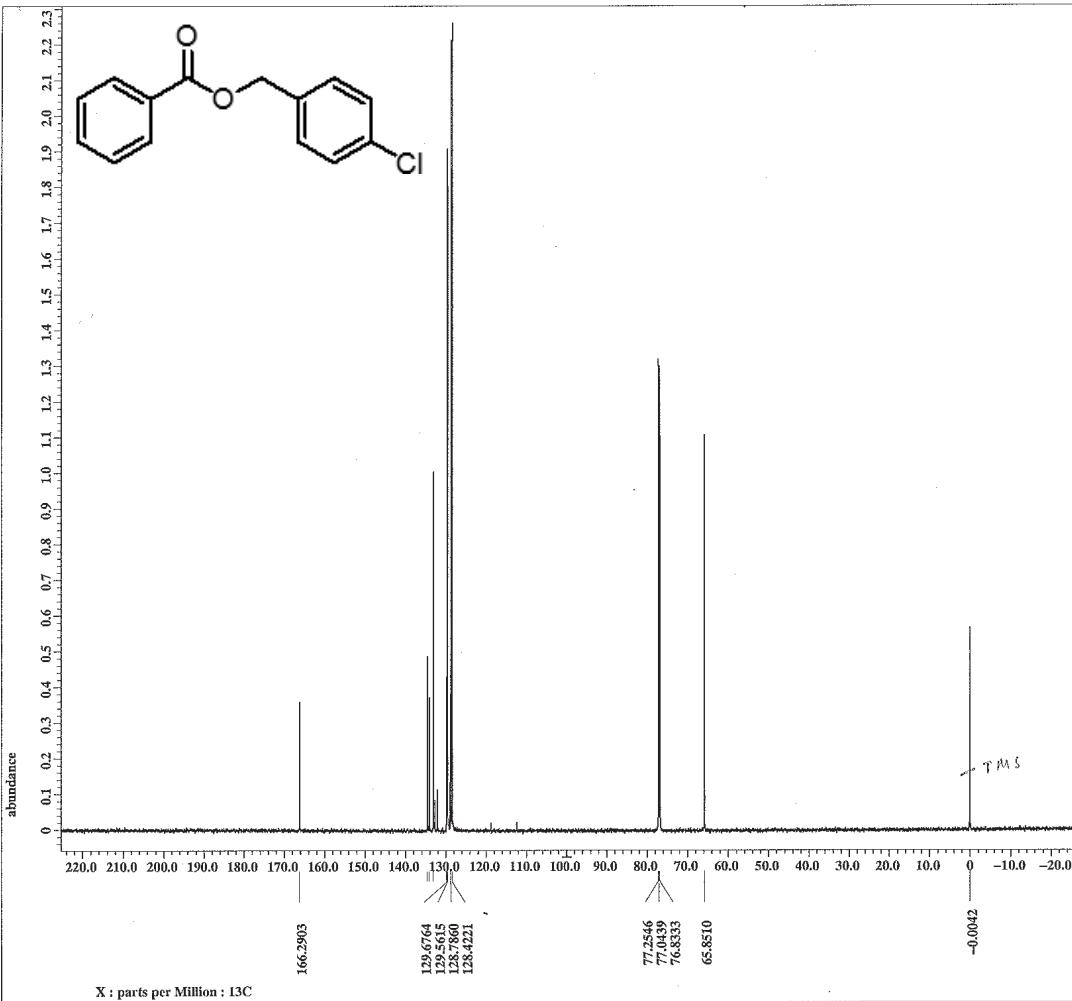
filename = Exp-AB-114-6-proton-5
author = delta
Experiment = single_pulse.ex3
Sample_id = Exp-AB-114-6-proton
Solvent = CHLOROFORM-D
Creation_time = 19-JUN-2014 20:55:14
Revision_time = 19-JUN-2014 22:23:02
Current_time = 19-JUN-2014 22:23:10

Content = Exp-AB-114-6-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 = 13[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atr = 3.6[dB]
X_pulse = 6[us]
Irr_atr = Off
Irr_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get = 20.9[dC]
  
```

X : parts per Million : 1H



JEOL

```

filename = Exp-AB-114-6-carbon-4
author = delta
Experiment = single_pulse_dec
Sample_id = Exp-AB-114-6-carbon
Solvent = CHLOROFORM-D
Creation_time = 19-JUN-2014 21:40:49
Revision_time = 25-JUN-2014 17:38:57
Current_time = 25-JUN-2014 17:39:24

Content = Exp-AB-114-6-carbon
Data_format = 1H 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 = 1000
Total_scans = 1000

X_90_width = 11.4[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atr = 7.5[dB]
X_pulse = 3.8[us]
Irr_atr_dec = 19.391[dB]
Irr_atr_noe = 19.391[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]
  
```

X : parts per Million : 13C

