

## Supporting information

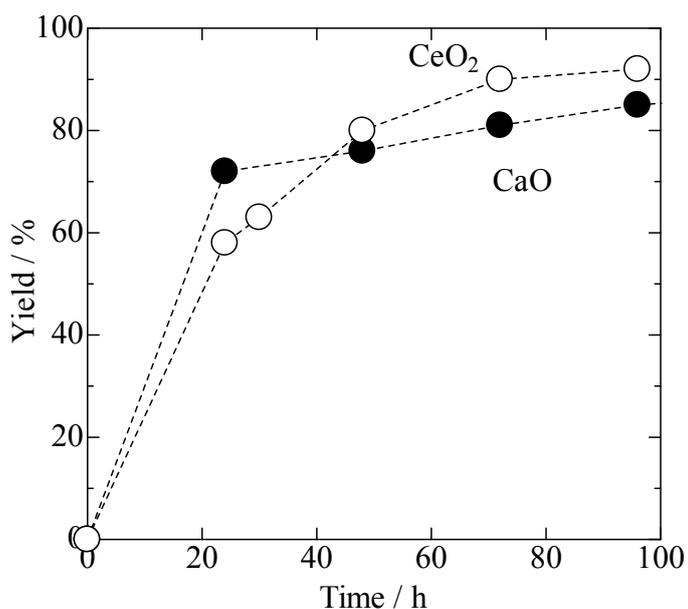
### CeO<sub>2</sub> as a versatile and reusable catalyst for transesterification of esters with alcohols under solvent-free conditions

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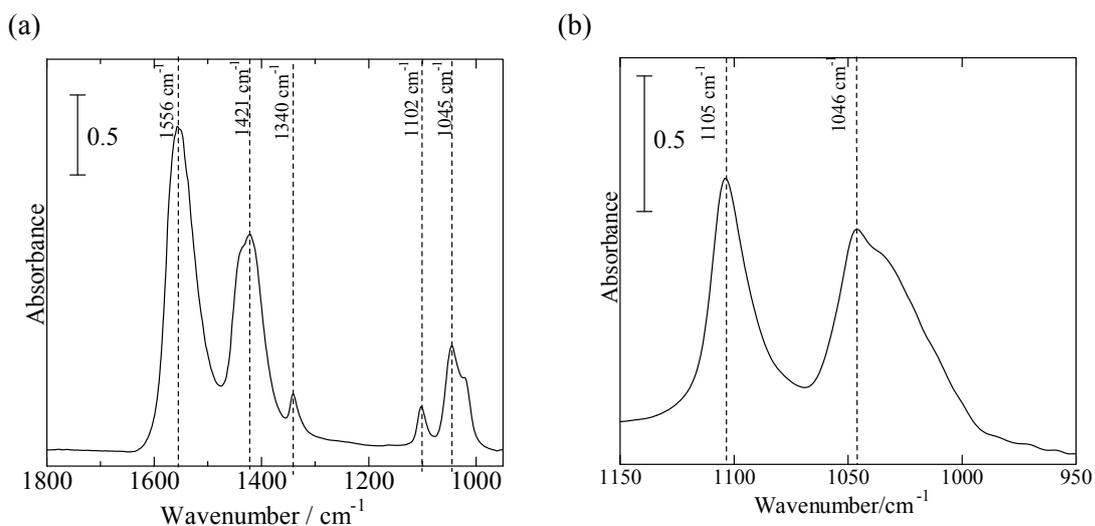
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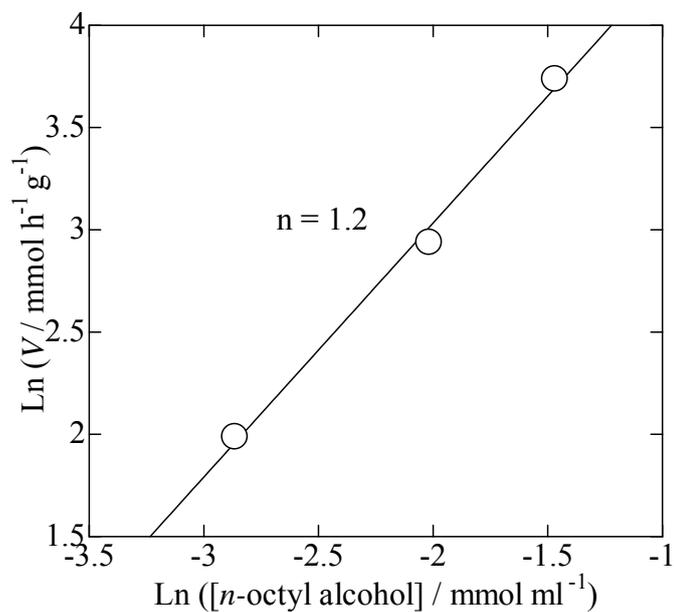
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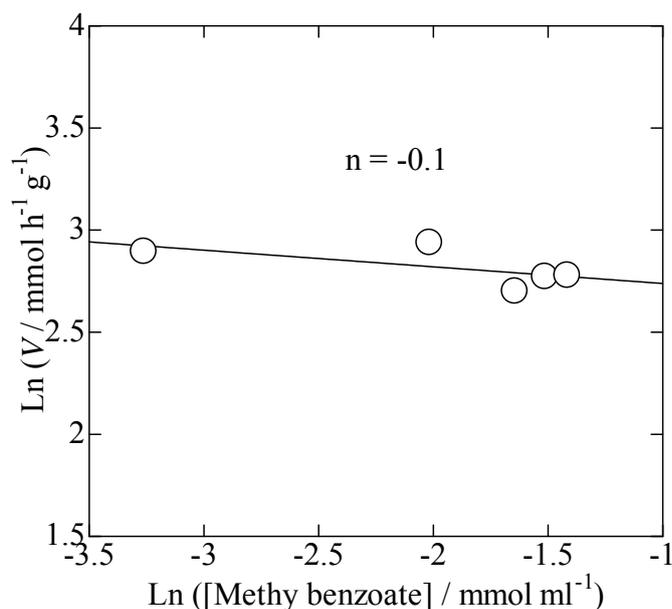
**Figure S1.** Yield of *n*-octyl benzoate vs time in the gram scale transesterification of methyl benzoate (12.5 mmol), *n*-octyl alcohol (15.4 mmol) by CaO or CeO<sub>2</sub> (50 mg) at 160 °C under open system.



**Figure S2.** *In-situ* IR spectra of adsorption complexes formed by introduction of 1  $\mu\text{L}$  of (a) methyl acetate or (b) methanol to  $\text{CeO}_2$ , followed by purging with He flow for 600 s at 30  $^\circ\text{C}$ .



**Figure S3.** Effect of the *n*-octyl alcohol concentration on the reaction rate (*V*). Reaction conditions: methyl benzoate (1.0 mmol), *n*-octyl alcohol (0.25 - 2 mmol), metal oxide (50 mg), *o*-xylene (0.5 g), reflux.

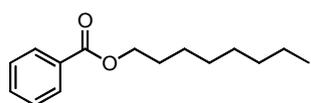


**Figure S4.** Effect of the concentration of methyl benzoate on the reaction rate ( $V$ ). Reaction conditions: methyl benzoate (0.25 - 2 mmol),  $n$ -octyl alcohol (1 mmol), metal oxide (50 mg),  $o$ -xylene (0.5 g), reflux.

### NMR and GC/MS analysis

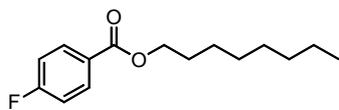
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for trans-esters of Table-3 and Table-4 were assigned and reproduced to the corresponding literature.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded using at ambient temperature on JEOL-ECX 600 operating at 600.17 and 150.92 MHz, respectively with tetramethylsilane as an internal standard. All chemical shifts ( $\delta$ ) are reported in ppm and coupling constants ( $J$ ) in Hz. All chemical shifts are reported relative to tetramethylsilane and  $d$ -solvent peaks (77.00 ppm, chloroform), 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.

### Data for Table-3



**Octyl benzoate (Product of T-3-Entry-1)<sup>1</sup>:**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  8.04 (d,  $J = 8.28$  Hz, 2H), 7.54 (t,  $J = 8.28$  Hz, 1H), 7.43 (t,  $J = 7.5$  Hz, 2H), 4.31 (t,  $J = 6.84$  Hz, 2H), 1.76 (m, 2H), 1.44 (m, 2H), 1.36-1.25 (m, 8H), 0.88 (t,  $J = 7.20$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  166.64, 132.74, 130.47, 129.48(C $\times$ 2), 128.26(C $\times$ 2), 65.09, 29.22(C $\times$ 2), 29.16, 28.67, 26.01, 22.61, 14.06; GC-MS  $m/e$  234.200.

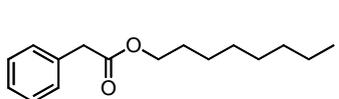
**Octyl 4-fluorobenzoate (Product of T-3-Entry-2)**<sup>2</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.06 (m, 2H), 7.11 (t



like, 2H), 4.30 (t, *J* = 6.9 Hz, 2H), 1.76 (m, 2H), 1.42 (m, 2H),  
1.39-1.22 (m, 8H), 0.89 (t, *J* = 7.20 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ

165.70, 165.64 (d, *J* = 254.31 Hz, 4-F-C), 132.01 (d, *J* = 8.66 Hz,  
meta to 4-F, C×2), 126.70, 115.40 (d, *J* = 21.67 Hz, ortho to 4-F, C×2), 65.26, 31.75, 29.21,  
29.16, 28.66, 25.99, 22.61, 14.06; GC-MS *m/e* 252.200.

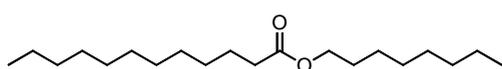
**Octyl 2-phenylacetate (Product of T-3-Entry-3)**<sup>3</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.13-7.28 (m, 5H), 4.07



(t, *J* = 6.48 Hz, 2H), 3.61 (s, 2H), 1.63 (m, 2H), 1.42-1.22 (m,  
10H), 0.88 (t, *J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 171.66,  
134.15, 129.20 (C×2), 128.48 (C×2), 126.97, 64.99, 41.44, 31.72,

29.11 (C×2), 28.50, 25.78, 22.60, 14.06; GC-MS *m/e* 248.200.

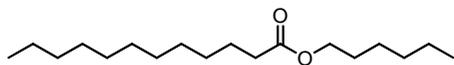
**Octyl dodecanoate (Product of T-3-entry-4)**<sup>4</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 4.06 (t, *J* = 6.9 Hz, 2H),



2.29 (m, 2H), 1.71-1.53 (m, 4H), 1.41-1.23 (m,  
26H), 0.89-0.88 (m, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ

174.02, 64.38, 31.89, 29.58 (C×4), 29.45 (C×3), 29.31, 29.26, 29.19, 29.17, 29.14, 25.91,  
22.62 (C×2), 14.07 (C×2); GC-MS *m/e* 298.350.

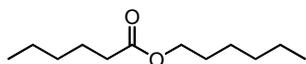
**Hexyl dodecanoate (Product of T-3-Entry-5)**<sup>5</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 4.05 (t, *J* = 6.84 Hz, 2H),



2.29 (m, 2H), 1.57 (m, 4H), 1.31-1.19 (m, 22 H),  
0.89-0.87 (m, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 174.03, 64.38,

34.39, 31.89 (C×2), 31.76, 31.42, 29.58 (C×2), 29.45, 29.32, 29.26, 29.20, 29.14, 28.62, 28.59,  
14.10, 13.98; GC-MS *m/e* 284.350.

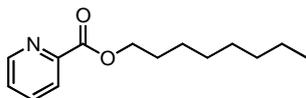
**Hexyl hexanoate (Product of T-3-Entry-6)**<sup>6</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 4.05 (t, *J* = 6.84 Hz, 2H),



2.29 (m, 2H), 1.55-1.51 (m, 4H), 1.38-1.29 (m, 10H), 0.89-0.88 (m,  
6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 173.96, 64.33, 34.31, 31.38, 31.28, 28.56,

25.55, 24.66, 22.50, 22.28, 13.94, 13.86; GC-MS *m/e* 186.200.

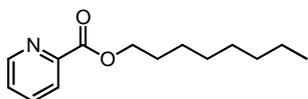
**Octyl picolinate (Product of T-3-Entry-7)**<sup>7</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.77 (d, *J* = 4.8 Hz, 1H), 8.13



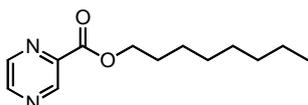
(d, *J* = 7.56 Hz, 1H), 7.85 (t like, 1H), 7.48 (t like, 1H), 4.41 (t, *J* =  
6.9 Hz, 2H), 1.83 (m, 2H), 1.43 (m, 2H), 1.38-1.22 (m, 8H), 0.87 (t,  
*J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 165.24, 149.85, 148.24,

136.91, 126.74, 125.04, 66.09, 31.73, 29.19, 29.11, 28.61, 25.85, 22.58, 14.04; GC-MS *m/e*  
235.150.

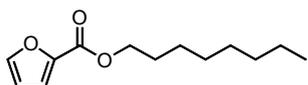
**Octyl picolinate (Product of T-3-Entry-8)**<sup>7</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.77 (d, *J* = 4.8 Hz, 1H), 8.13 (d, *J* = 7.56 Hz, 1H), 7.85 (t like, 1H), 7.48 (t like, 1H), 4.41 (t, *J* = 6.9 Hz, 2H), 1.82 (m, 2H), 1.43 (m, 2H), 1.36-1.22 (m, 8H), 0.87 (t, *J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 165.24, 149.85, 148.24, 136.91, 126.74, 125.04, 66.09, 31.73, 29.19, 29.11, 28.61, 25.85, 22.58, 14.04; GC-MS *m/e* 235.150.



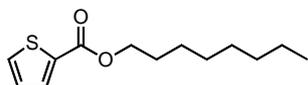
**Octyl pyrazine-2-carboxylate (Product of T-3-Entry-9)**<sup>8</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 9.31 (s, 1H), 8.77 (d like, 1H), 8.75 (d like, 1H), 4.45 (t, *J* = 6.9 Hz, 2H), 1.83 (m, 2H), 1.44 (m, 2H), 1.36-1.22 (m, 8H), 0.88 (t, *J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 163.94, 147.53, 146.22, 144.42, 143.58, 66.50, 31.71, 29.14, 29.10, 28.54, 25.82, 25.58, 14.04; GC-MS *m/e* 236.150.



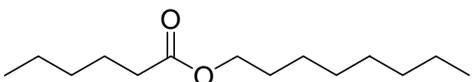
**Octyl furan-2-carboxylate (Product of T-3-Entry-10)**<sup>9</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.57 (s, 1H), 7.17 (d, *J* = 3.42 Hz, 1H), 6.50 (m, 1H), 4.30 (t, *J* = 6.78 Hz, 2H), 1.73 (m, 2H), 1.40 (m, 2H), 1.38-1.22 (m, 8H), 0.88 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 158.84, 146.12, 144.84, 117.64, 111.73, 65.08, 31.73, 29.16, 29.12, 28.63, 25.85, 22.59, 14.04; GC-MS *m/e* 224.140.



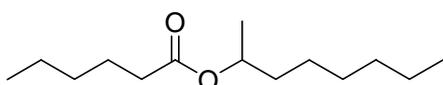
**Thiophene-2-carboxylic acid octyl ester (Product of T-3-Entry-11)**<sup>10</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.80 (d, *J* = 4.14 Hz, 1H), 7.54 (d, *J* = 4.80 Hz, 1H), 7.09 (t, *J* = 4.3 Hz, 1H), 4.28 (t, *J* = 6.54 Hz, 2H), 1.75-1.72 (m, 2H), 1.42-1.38 (m, 2H), 1.34-1.26 (m, 8H), 0.88 (t, *J* = 6.87 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 162.30, 134.06, 133.16, 132.10, 127.63, 65.26, 31.74, 29.17, 29.14, 28.63, 25.90, 22.60, 14.05; GC-MS *m/e* 240.100.



**Hexanoic acid octyl ester (Product of T-3-Entry 12)**<sup>20</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 4.05 (t, *J* = 6.51, Hz, 2H), 2.29 (t, *J* = 7.53 Hz, 2H), 1.63-1.60 (m, 4H), 1.31-1.28 (m, 14H), 0.89-0.87 (m, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 173.97, 64.36, 34.33, 31.74, 31.29, 29.18, 29.16, 28.61, 25.89, 24.68, 22.60, 22.29, 14.04, 13.88; GC-MS *m/e* 228.380.

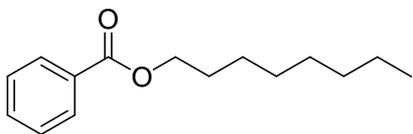


**Hexanoic acid 1-methyl-heptyl ester (Product of T-3-Entry 13)**<sup>20</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 4.89 (m, 1H), 2.26 (t, *J* = 7.56 Hz, 2H), 1.63-1.55 (m, 3H), 1.46 (m, 1H), 1.36-1.22 (m, 12 H), 1.19 (d, *J* = 6.84 Hz, 3H), 0.89-0.87 (m, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 173.54,

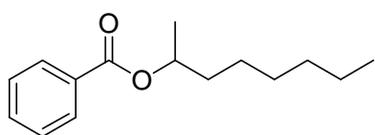


70.67, 35.93, 34.68, 31.72, 31.29, 29.07, 25.34, 24.76, 22.54, 22.30, 19.99, 14.02, 13.88;  
GC-MS *m/e* 228.360.

**Octyl benzoate (Product of T-3-Entry-14)<sup>1</sup>:** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.04 (d, *J* = 8.28 Hz, 2H), 7.54 (t, *J* = 8.28 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 4.31 (t, *J* = 6.84 Hz, 2H), 1.76 (m, 2H), 1.44 (m, 2H), 1.36-1.25 (m, 8H), 0.88 (t, *J* = 7.20 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.64, 132.74, 130.47, 129.48(C×2), 128.26(C×2), 65.09, 29.22(C×2), 29.16, 28.67, 26.01, 22.61, 14.06; GC-MS *m/e* 234.200.

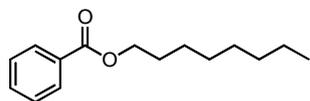


**Benzoic acid 1-methyl-heptyl ester (Product of T-3-Entry-15)<sup>3</sup>:** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.04 (d, *J* = 8.26 Hz, 2H), 7.53 (t, *J* = 7.54 Hz, 1H), 7.33 (t, *J* = 7.54 Hz, 2H), 5.14 (m, 1H), 1.73 (m, 1H), 1.60 (m, 1H), 1.45- 1.26 (m, 11H), 0.87 (t, *J* = 7.25 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.13, 132.59, 130.86, 129.43, 128.19, 71.64, 36.01, 31.68, 29.10, 25.35, 22.52, 20.01, 14.01; GC-MS *m/e* 234.200.

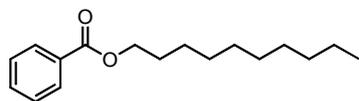


#### Data for Table-4

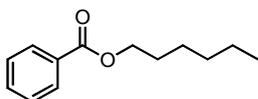
**Octyl benzoate (Product of T-4-Entry-1)<sup>1</sup>:** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.04 (d, *J* = 8.28 Hz, 2H), 7.54 (t, *J* = 8.28 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 4.31 (t, *J* = 6.84 Hz, 2H), 1.76 (m, 2H), 1.44 (m, 2H), 1.36-1.25 (m, 8H), 0.88 (t, *J* = 7.20 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.64, 132.74, 130.47, 129.48(C×2), 128.26(C×2), 65.09, 29.22(C×2), 29.16, 28.67, 26.01, 22.61, 14.06; GC-MS *m/e* 234.200.



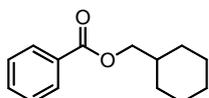
**Benzoic acid decyl ester (Product of T-4-Entry-2)<sup>11</sup>:** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.04 (d, *J* = 6.9 Hz, 2H), 7.55 (t, *J* = 7.56 Hz, 1H), 7.43 (t, *J* = 7.56 Hz, 2H), 4.31 (t, *J* = 6.48 Hz, 2H), 1.76 (m, 2H), 1.44 (m, 2H), 1.36-1.22 (m, 12H), 0.88 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.66, 132.75, 130.48, 129.48(C×2), 128.27(C×2), 65.11, 31.86, 29.50(C×2), 29.27, 29.26, 28.68, 26.01, 22.65, 14.09; GC-MS *m/e* 262.350.



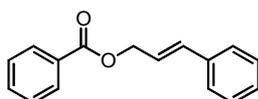
**Hexyl benzoate (Product of T-4-Entry-3)**<sup>12</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.05 (d, *J* = 8.28 Hz, 2H), 7.54 (t, *J* = 7.56 Hz, 1H), 7.43 (t, *J* = 7.56 Hz, 2H), 4.30 (t, *J* = 6.9 Hz, 2H), 1.76 (m, 2H), 1.44 (m, 2H), 1.38-1.32 (m, 4H), 0.90 (t, *J* = 6.54 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.64, 132.74, 130.47, 129.48(C×2), 128.26(C×2), 65.08, 31.43, 28.63, 25.67, 22.51, 13.98; GC-MS *m/e* 206.250.



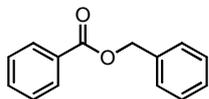
**Cyclohexylmethyl benzoate (Product of T-4-Entry-5)**<sup>13</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.05 (d, *J* = 8.22 Hz, 2H), 7.55 (t, *J* = 7.56 Hz, 1H), 7.43 (t, *J* = 7.56 Hz, 2H) 4.12 (t, *J* = 6.9 Hz, 2H), 1.84 (m, 2H), 1.81-1.75 (m, 3H), 1.69 (m, 1H), 1.28 (m, 2H), 1.20 (m, 1H), 1.07 (m, 2H), ; <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.63, 132.75, 130.49, 129.48(C×2), 128.28(C×2), 70.02, 37.22, 29.71(C×2), 26.33, 25.67(C×2); GC-MS *m/e* 218.250.



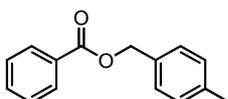
**Cinnamyl benzoate (Product of T-4-Entry-6)**<sup>14</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.09 (d, *J* = 7.86 Hz, 2H), 7.57-7.53 (m, 2H), 7.46-7.42 (m, 2H), 7.36-7.32 (m, 2H), 7.28-7.7.24 (m, 2H), 6.74 (d, *J* = 15.84 Hz, 1H), 6.41 (m, 1H), 4.99 (d, *J* = 6.18 Hz, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.38, 136.22, 134.22, 132.98, 129.62(C×2), 128.58(C×2), 128.47, 128.33(C×2), 128.06, 126.60(C×2), 123.19, 65.52; GC-MS *m/e* 238.250.



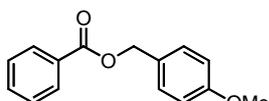
**Benzyl benzoate (Product of T-4-Entry-7)**<sup>15</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.08 (d, *J* = 4.56 Hz, 2H), 7.54 (t, *J* = 7.56 Hz, 1H), 7.45-7.41 (m, 4H), 7.39-7.32 (m, 3H) 5.36 (s, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.39, 135.99, 133.0, 130.06, 129.66(C×2), 128.56(C×2), 128.33(C×2), , 128.20, 128.12(C×2), 66.65; GC-MS *m/e* 212.200.



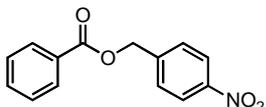
**4-methylbenzyl benzoate (Product of T-4-Entry-8)**<sup>16</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.06 (d, *J* = 8.28 Hz, 2H), 7.54 (t, *J* = 7.92 Hz, 1H), 7.42 (t, *J* = 7.92 Hz, 2H), 7.35 (d, *J* = 8.22 Hz, 2H), 7.19 (d, *J* = 8.22 Hz, 2H), 5.32 (s, 2H), 2.35 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.45, 138.05, 132.98, 132.93, 130.15, 129.65(C×2), 129.23(C×2), 128.33(C×2), 128.30(C×2), 66.63, 21.19; GC-MS *m/e* 226.150.



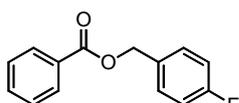
**4-methoxybenzyl benzoate (Product of T-4-Entry-9)**<sup>17</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.05 (d, *J* = 7.56 Hz, 2H), 7.58 (t, *J* = 7.56 Hz, 1H), 7.42-7.38 (m, 4H), 6.90 (d, *J* = 8.22 Hz, 2H), 5.29 (s, 2H), 3.79 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.46, 159.57, 132.89, 130.17, 130.02(C×2), 129.60(C×2), 128.27 (C×2), 128.08, 113.89 (C×2), 66.48, 55.22; GC-MS *m/e* 242.200.



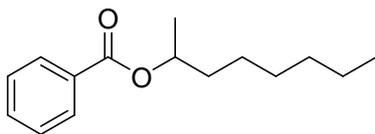
**4-nitro benzoate (Product of T-4-Entry-10)<sup>18</sup>:** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.24 (d, *J* = 8.22 Hz, 2H), 8.09 (d, *J* = 7.56 Hz, 2H), 7.62-7.59 (m, 3H), 7.47 (t, *J* = 7.56 Hz, 2H), 5.46 (s, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.06, 147.84, 143.29, 133.42, 129.66(C×2), 128.50(C×2), 128.25(C×2), 126.90, 123.79(C×2), 65.11; GC-MS *m/e* 257.150.



**Benzoic acid 4-fluoro-benzyl ester (Product of T-4-Entry-11)<sup>19</sup>:** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.06 (d, *J* = 7.56 Hz, 2H), 7.55 (t, *J* = 7.56 Hz, 1H), 7.44-7.41 (m, 4H), 7.06 (t, *J* = 8.58 Hz, 2H), 5.32 (s, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.33, 162.61 (d, *J* = 247.49 Hz, 4-F-C), 133.07, 131.84(C×2), 130.19, 130.14, 129.93, 129.63(C×2), 128.36(C×2), 115.48(d, *J* = 21.67 Hz, ortho to 4-F), 65.94; GC-MS *m/e* 230.150.



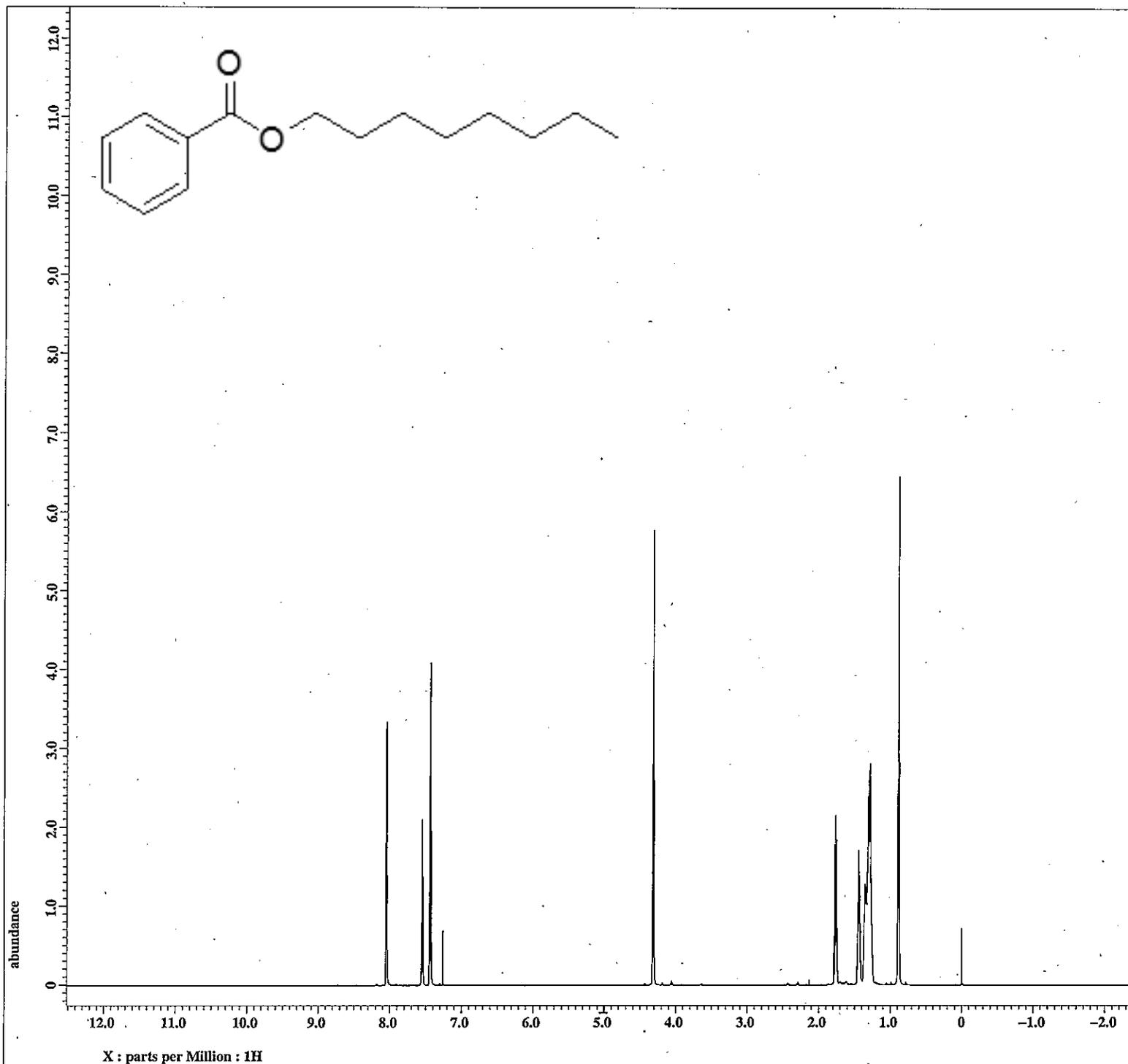
**Benzoic acid 1-methyl-heptyl ester (Product of T-4-Entry-12)<sup>3</sup>:** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.04 (d, *J* = 8.26 Hz, 2H), 7.53 (t, *J* = 7.54 Hz, 1H), 7.33 (t, *J* = 7.54 Hz, 2H), 5.14 (m, 1H), 1.73 (m, 1H), 1.60 (m, 1H), 1.45-1.26 (m, 11H), 0.87 (t, *J* = 7.25 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 166.13, 132.59, 130.86, 129.43, 128.19, 71.64, 36.01, 31.68, 29.10, 25.35, 22.52, 20.01, 14.01; GC-MS *m/e* 234.200.



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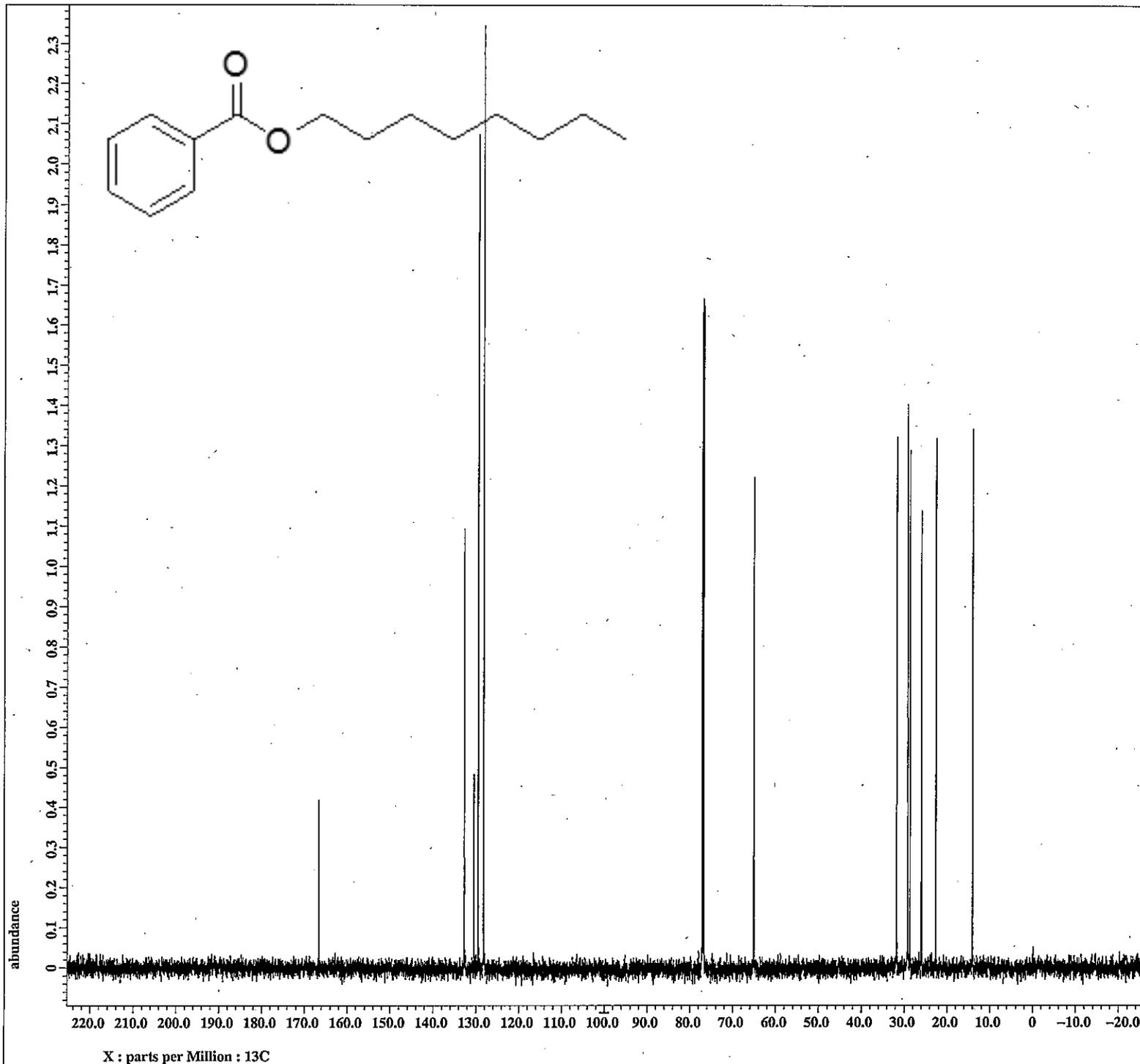


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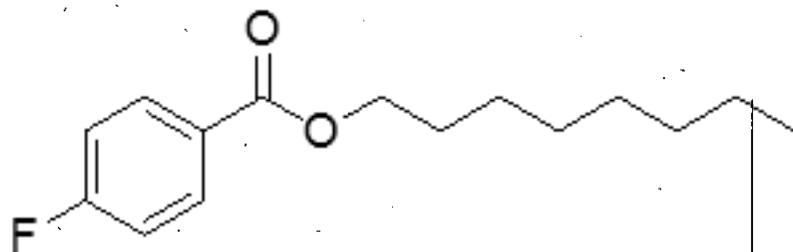
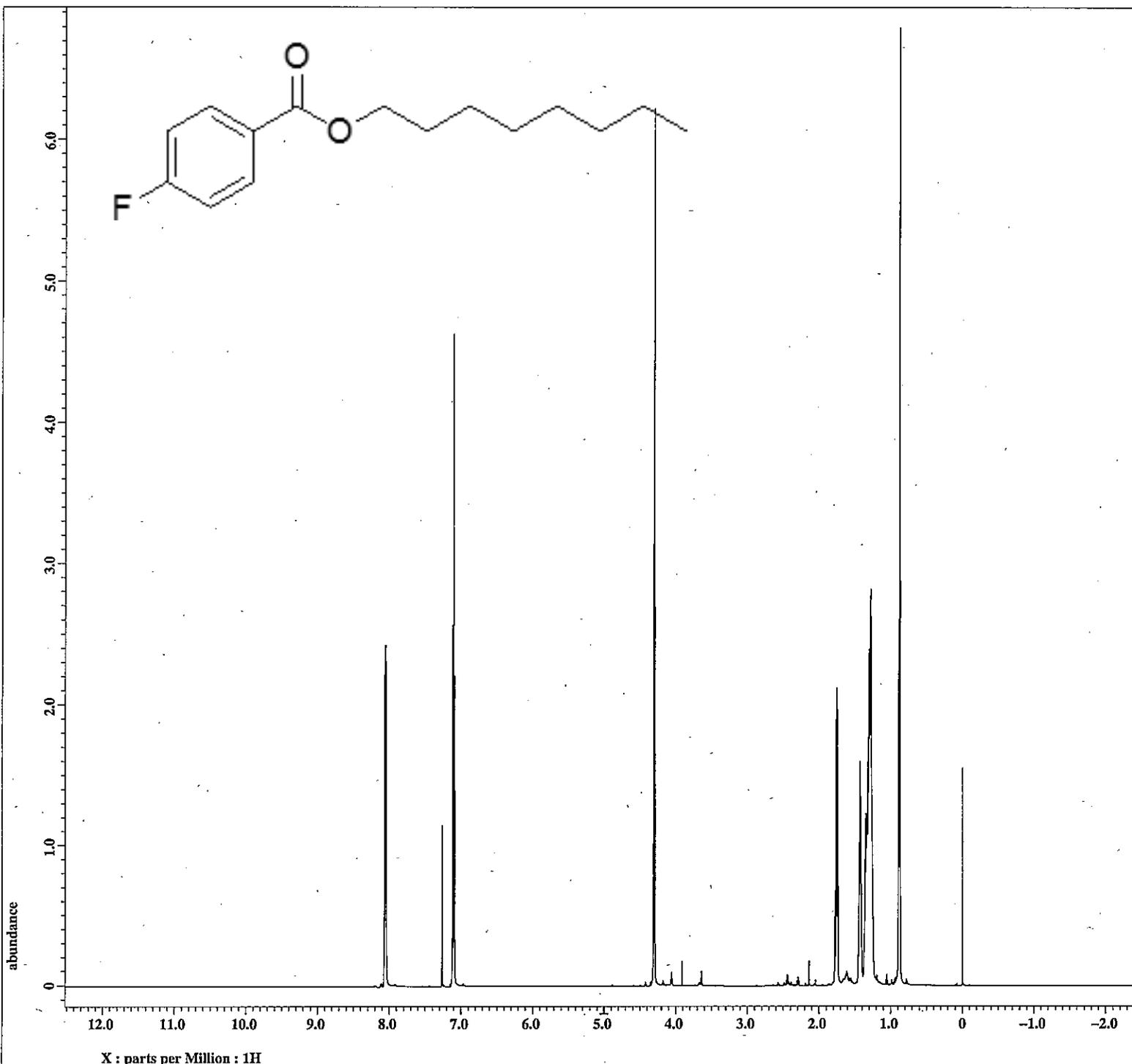


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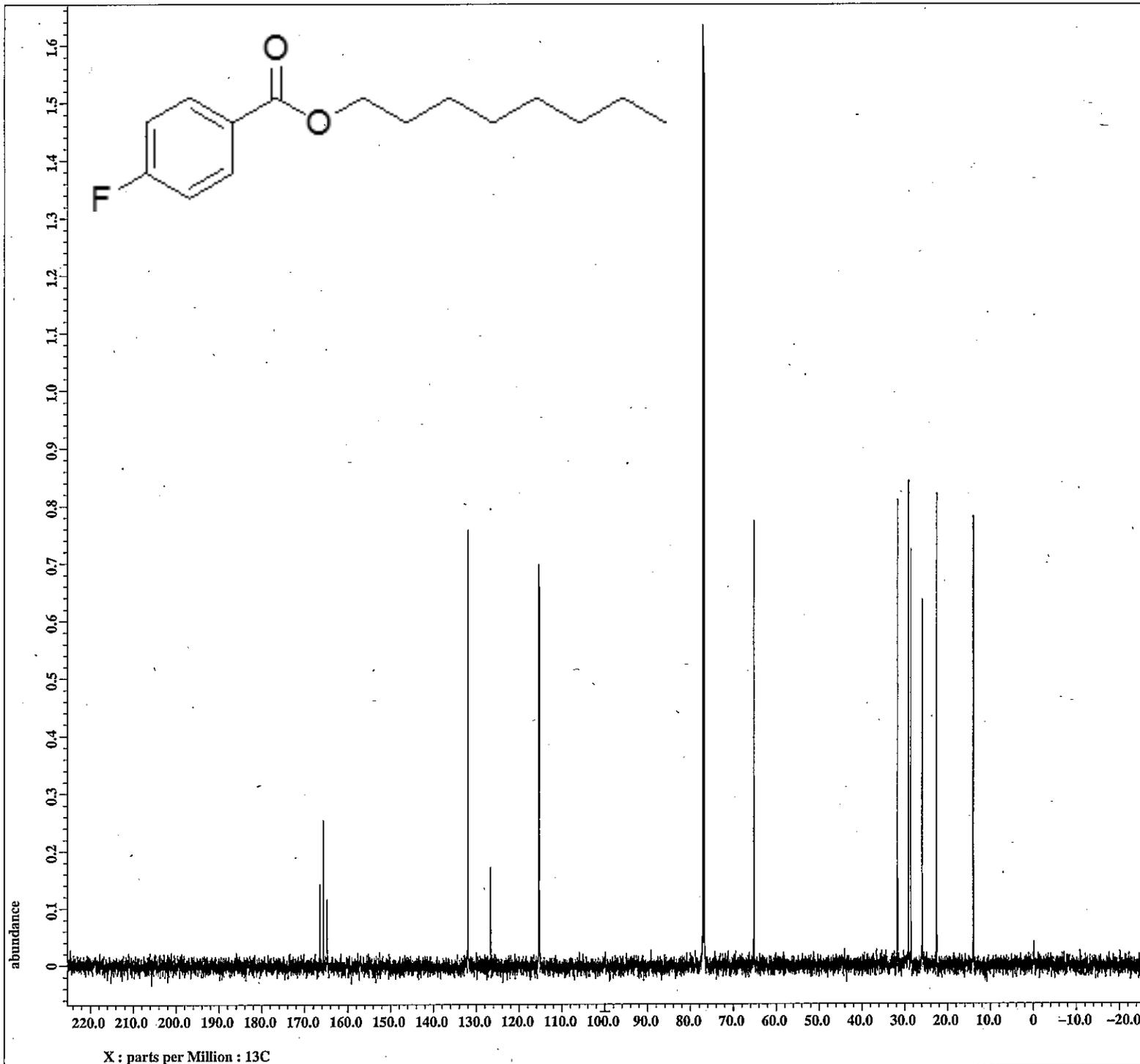


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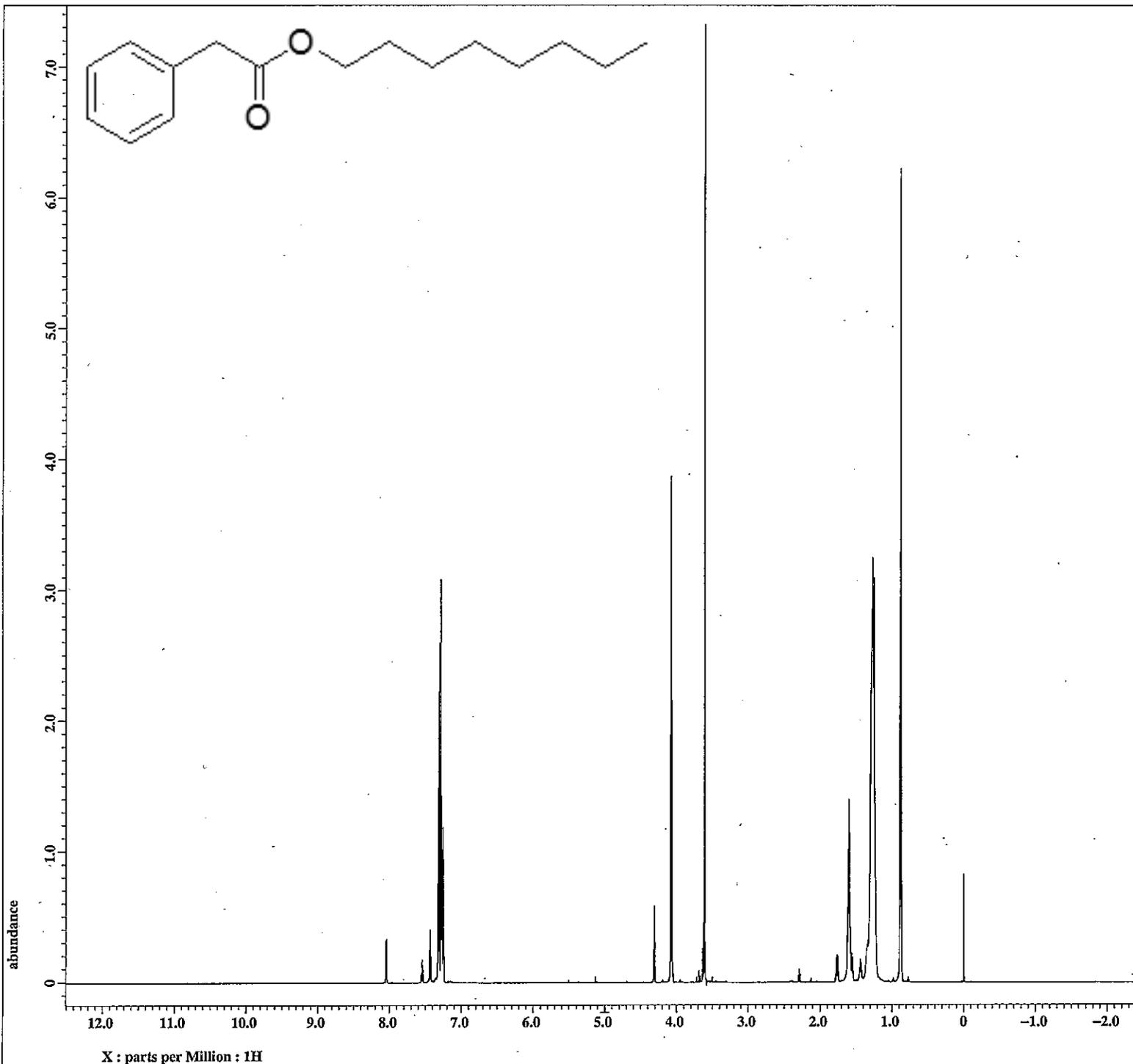


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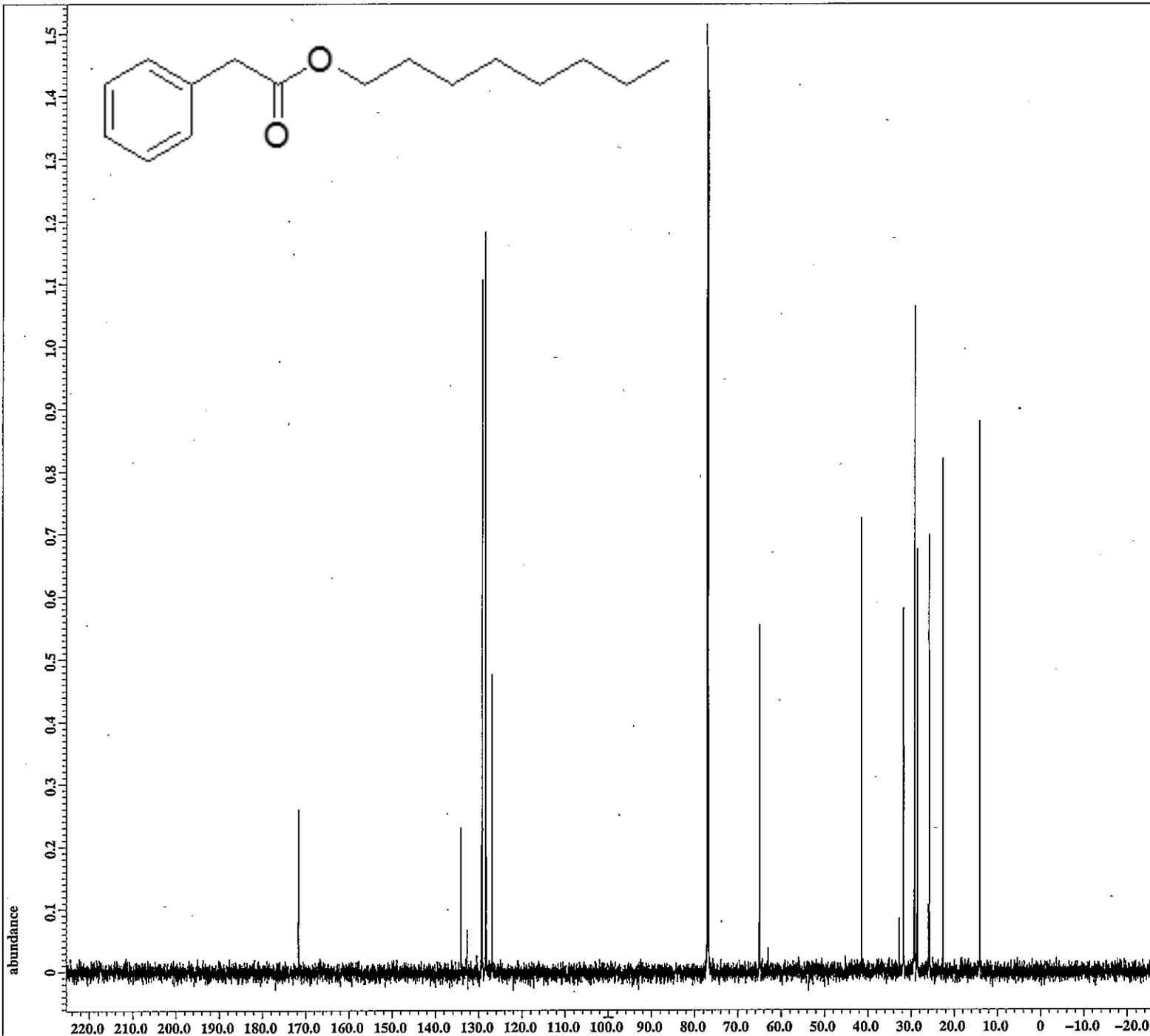
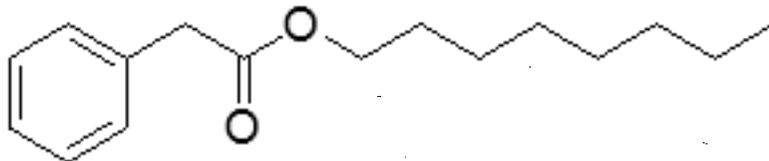


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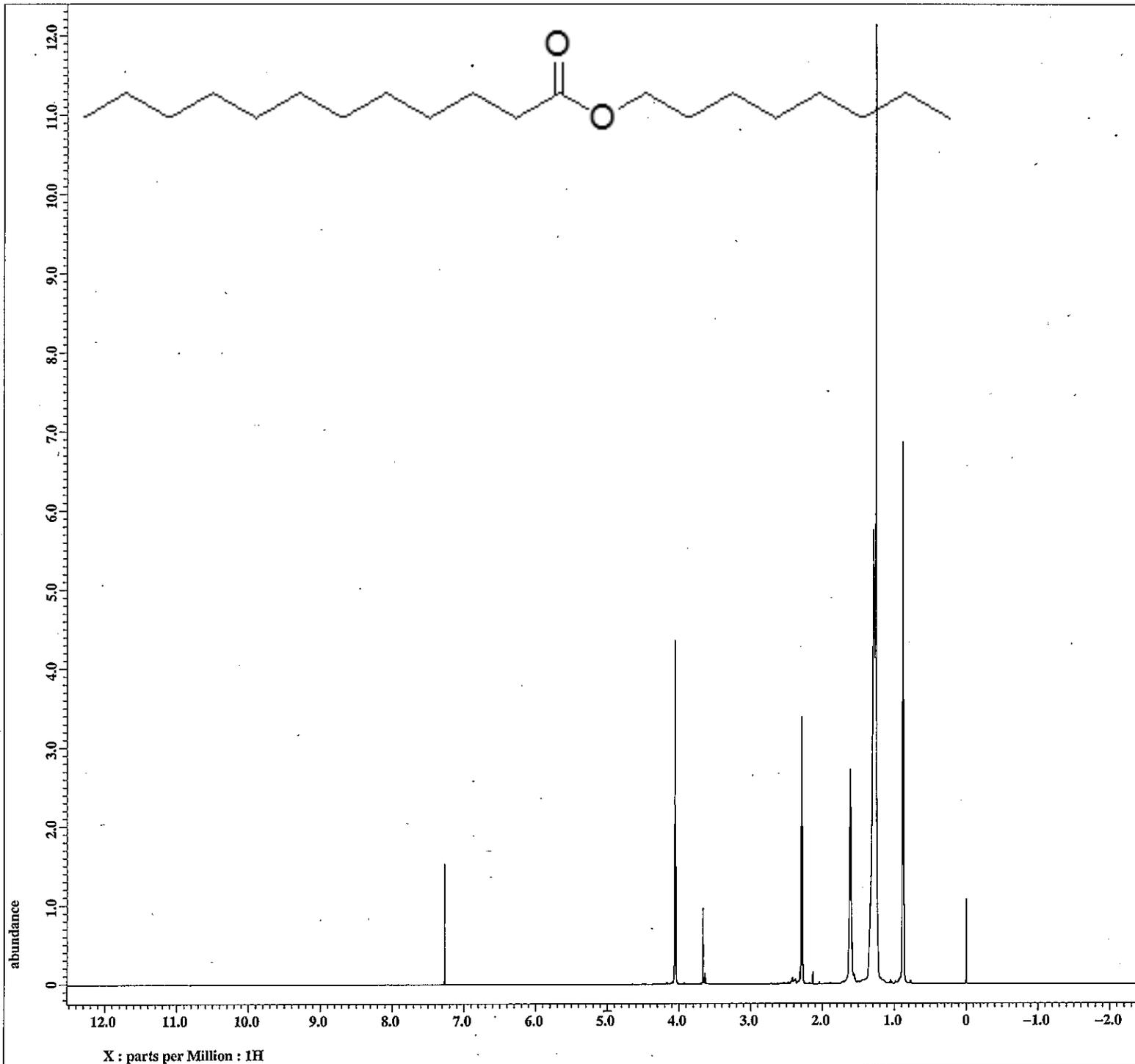
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X : parts per Million : 13C

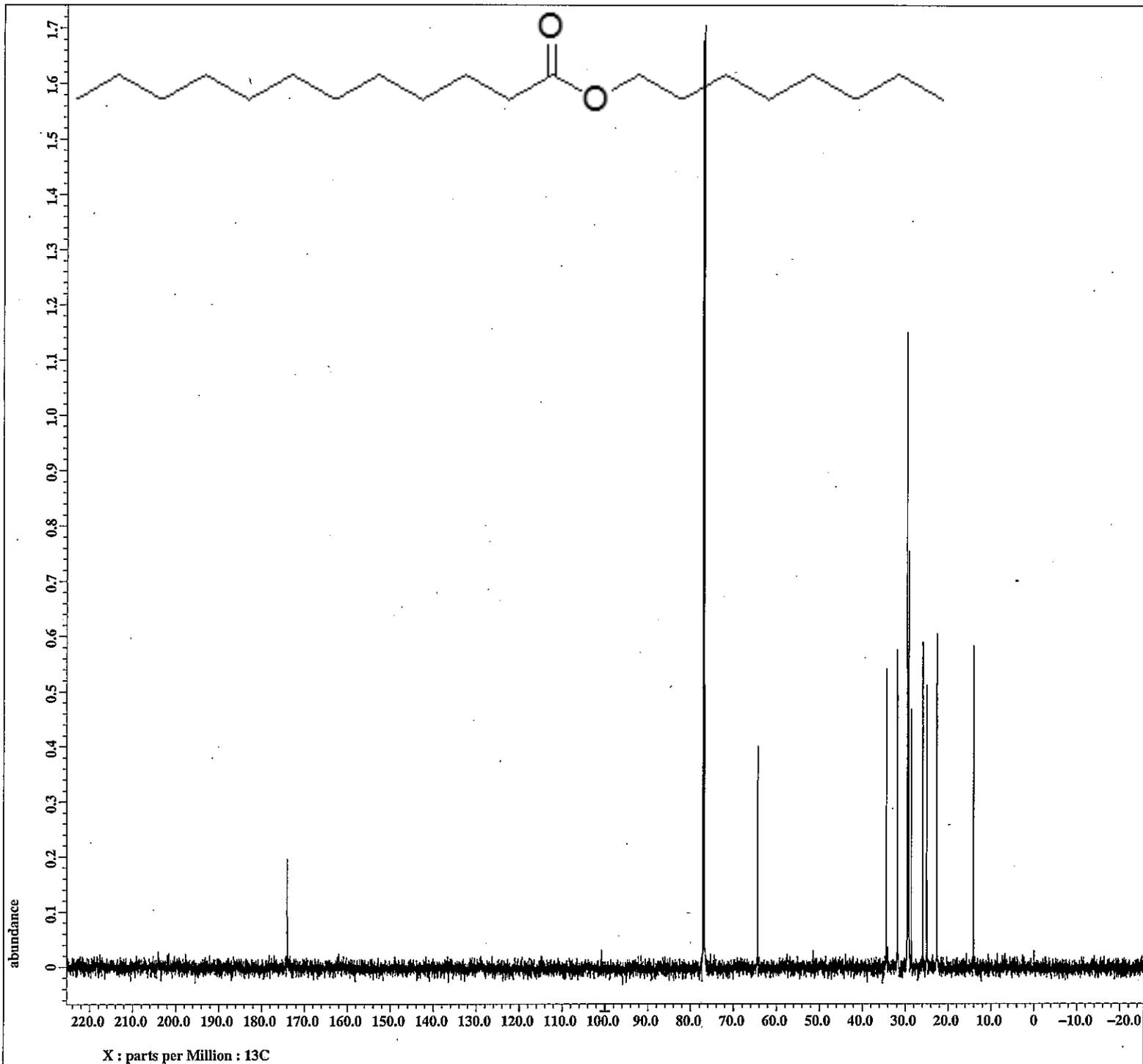


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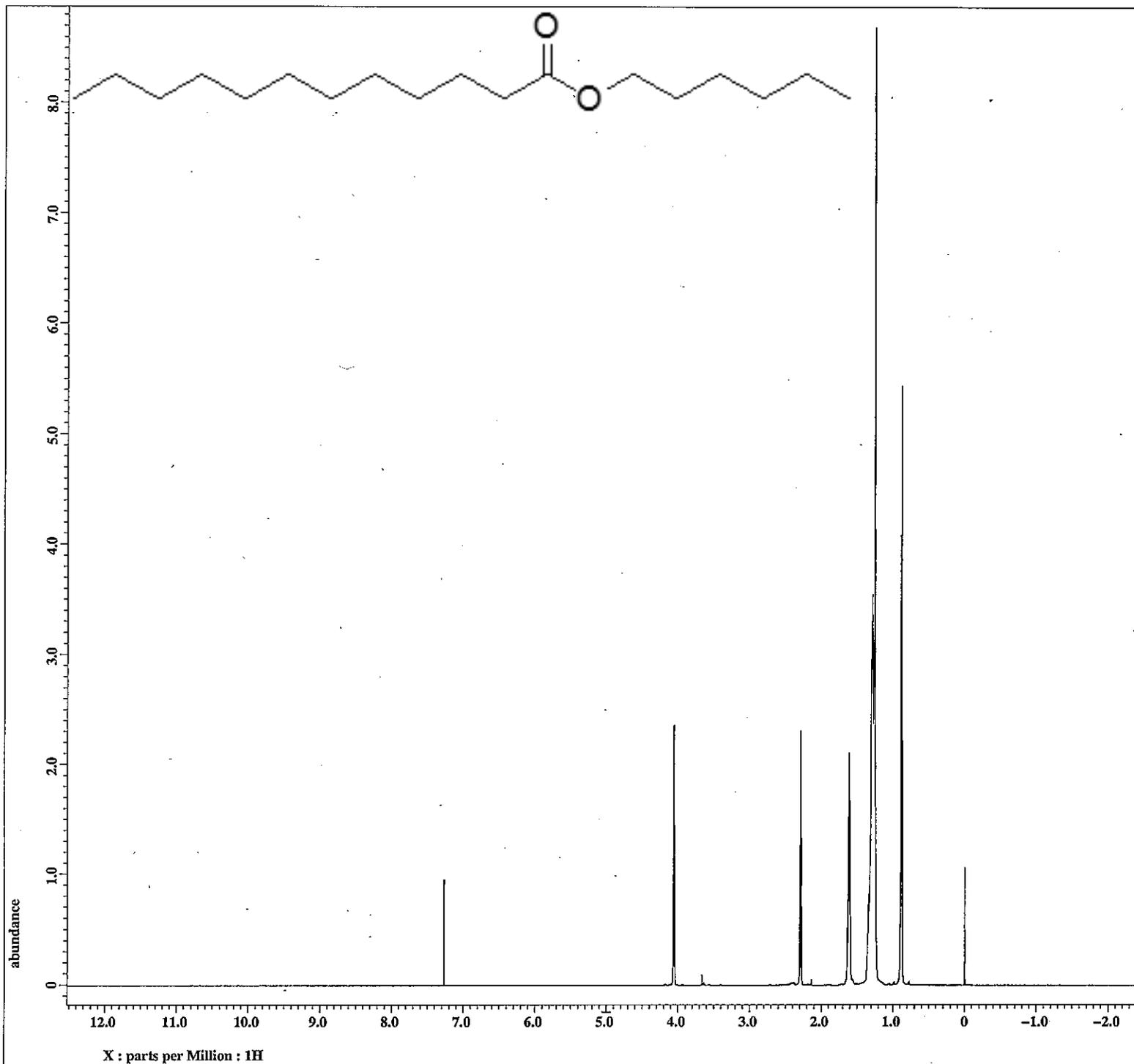


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Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 20:35:26  
Revision\_time = 5-DEC-2012 20:21:05  
Current\_time = 5-DEC-2012 20:21:12

Content = Exp-T-3-4-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 124  
Total\_scans = 124

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[dB]  
Irr\_noise = WALTZ  
Decoupling = TRUE  
Initial\_wait = 1[s]  
Noe = TRUE  
Noe\_time = 2[s]  
Recvr\_gain = 60  
Relaxation\_delay = 2[s]  
Repetition\_time = 2.69206016[s]  
Temp\_get = 20.1[dC]

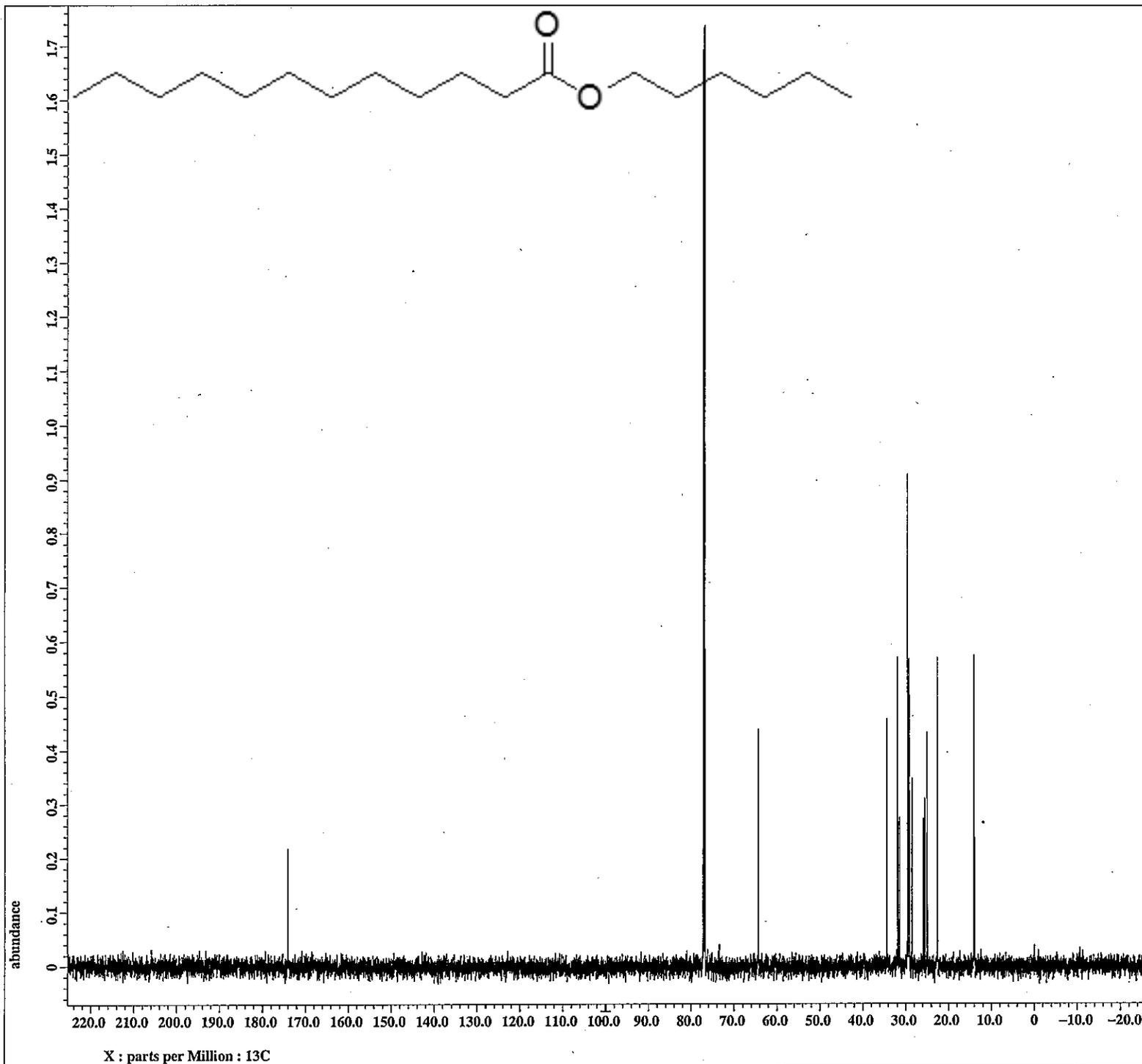


Filename = Exp-T-3-5-proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-T-3-5-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 20:44:25  
Revision\_time = 5-DEC-2012 20:29:44  
Current\_time = 5-DEC-2012 20:29:51

Content = Exp-T-3-5-proton  
Data\_format = 1D\_COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 40  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 18.9[degC]

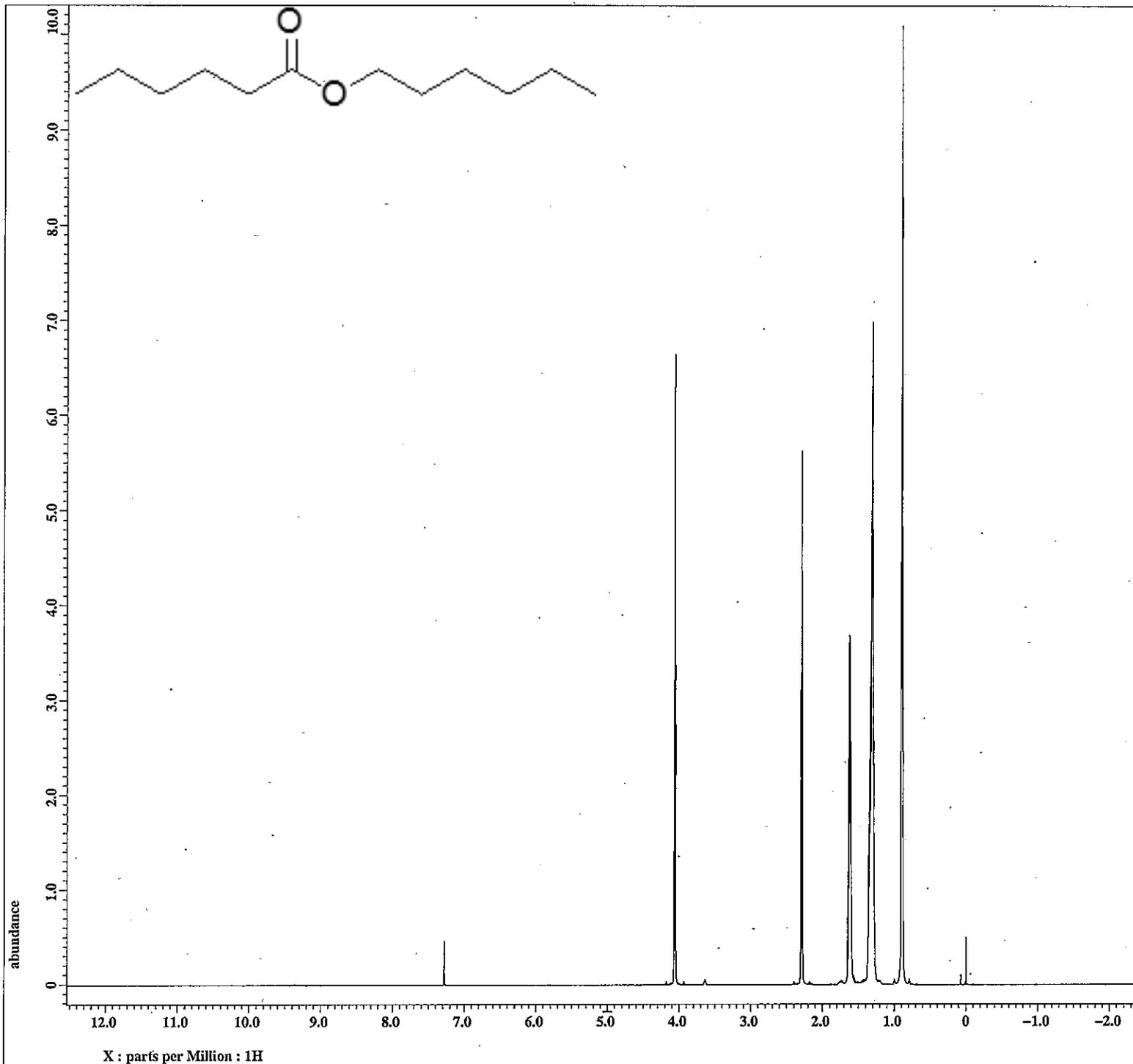


Filename = Exp-T-3-5-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-3-5-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 20:48:36  
Revision\_time = 5-DEC-2012 20:30:36  
Current\_time = 5-DEC-2012 20:30:42

Content = Exp-T-3-5-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039 [MHz]  
X\_offset = 100 [ppm].  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109 [Hz]  
X\_sweep = 47.34848485 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 77  
Total\_scans = 77

X\_90\_width = 11.3 [us]  
X\_acq\_time = 0.69206016 [s]  
X\_angle = 30 [deg]  
X\_atn = 8 [dB]  
X\_pulse = 3.76666667 [us]  
Irr\_atn\_dec = 19.34784 [dB]  
Irr\_atn\_noe = 19.34784 [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 = 19.6 [dC]

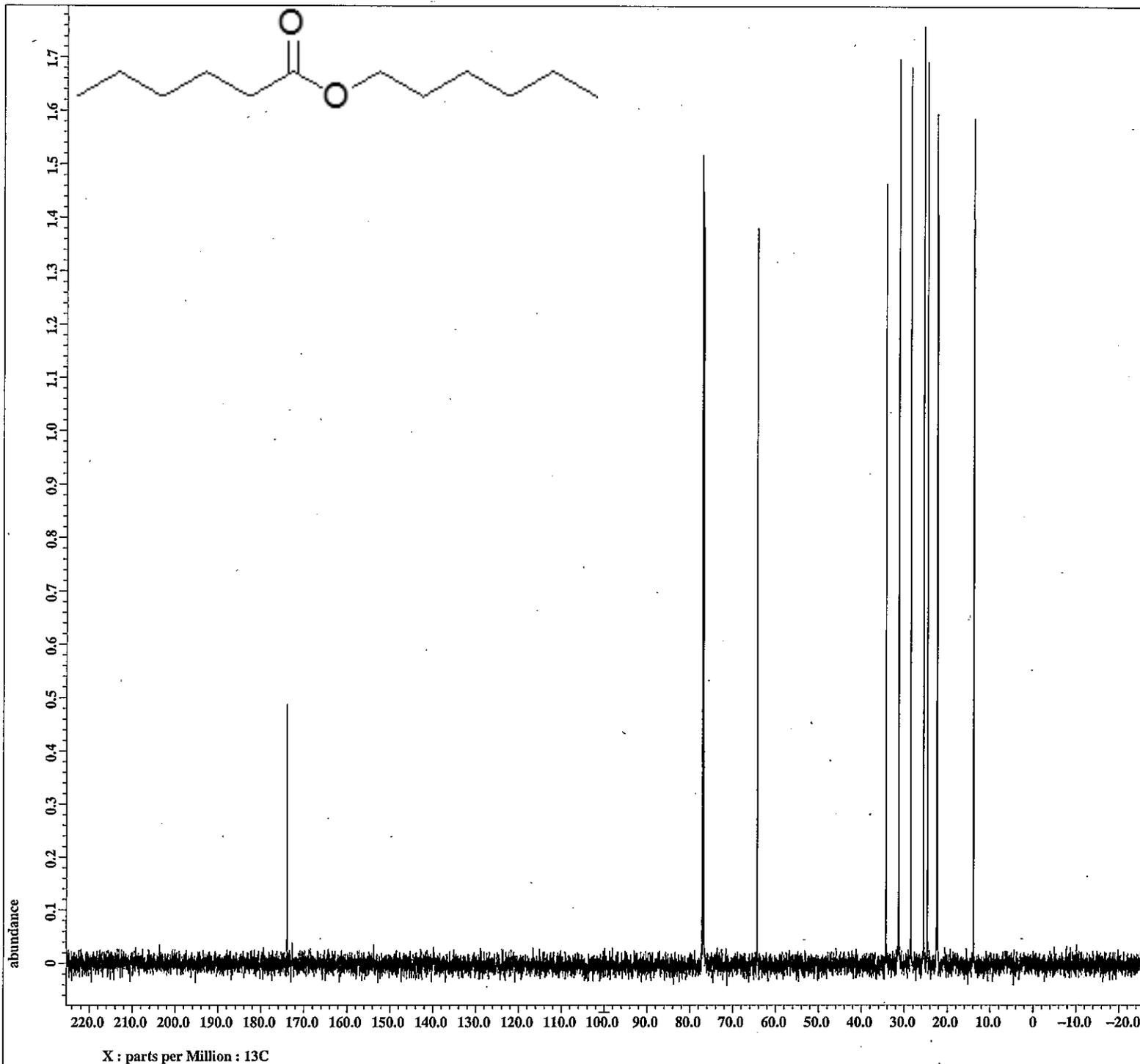


Filename = Exp-T-3-6-proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-T-3-6-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 20:57:57  
Revision\_time = 5-DEC-2012 20:31:21  
Current\_time = 5-DEC-2012 20:31:26

Content = Exp-T-3-6-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 = TRUE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 36  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.4[dc]

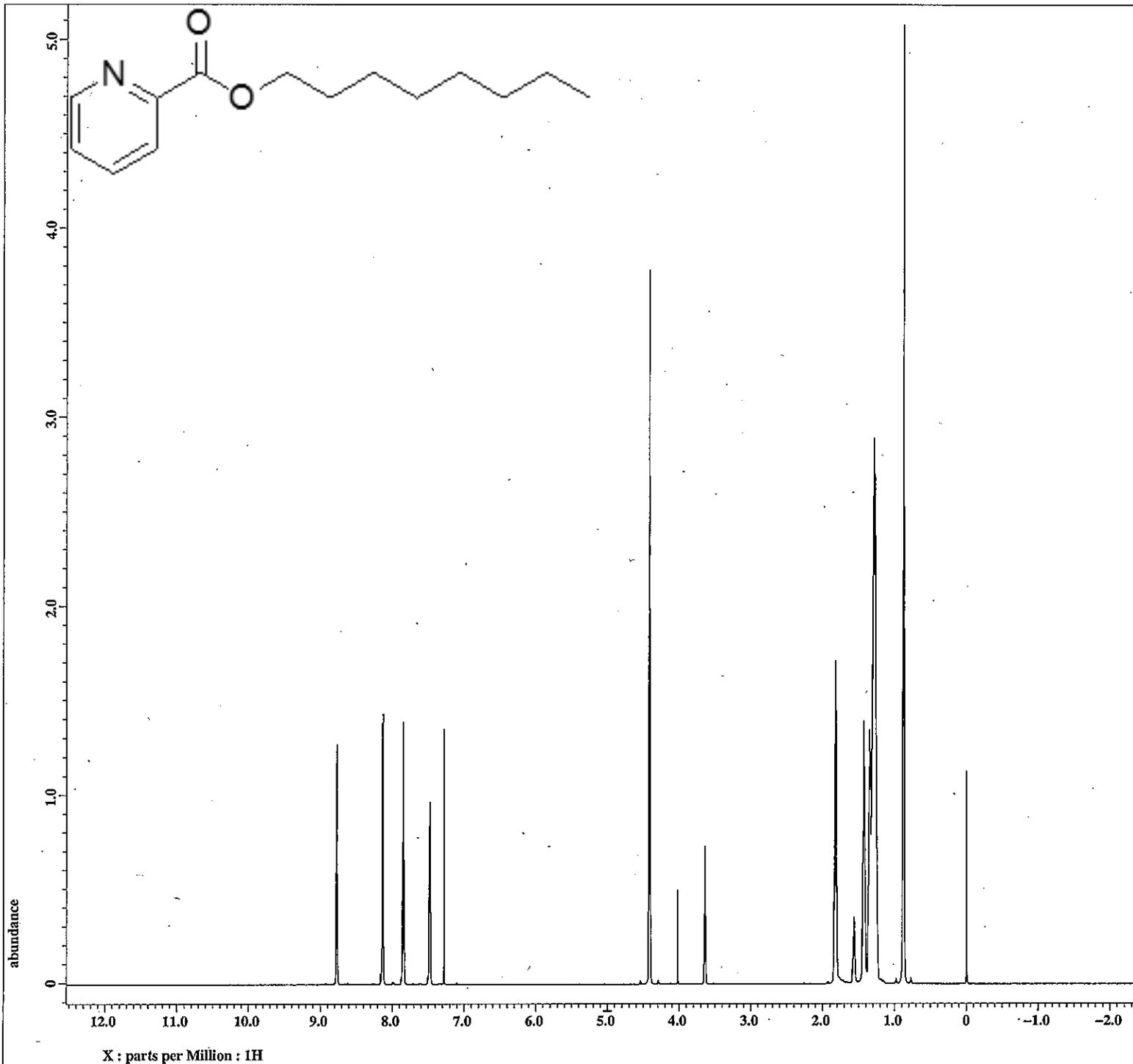


Filename = Exp-T-3-6-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-3-6-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:01:37  
Revision\_time = 5-DEC-2012 20:32:00  
Current\_time = 5-DEC-2012 20:32:09

Content = Exp-T-3-6-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 66  
Total\_scans = 66

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[db]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[db]  
Irr\_atn\_noe = 19.34784[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 = 19.7[dc]

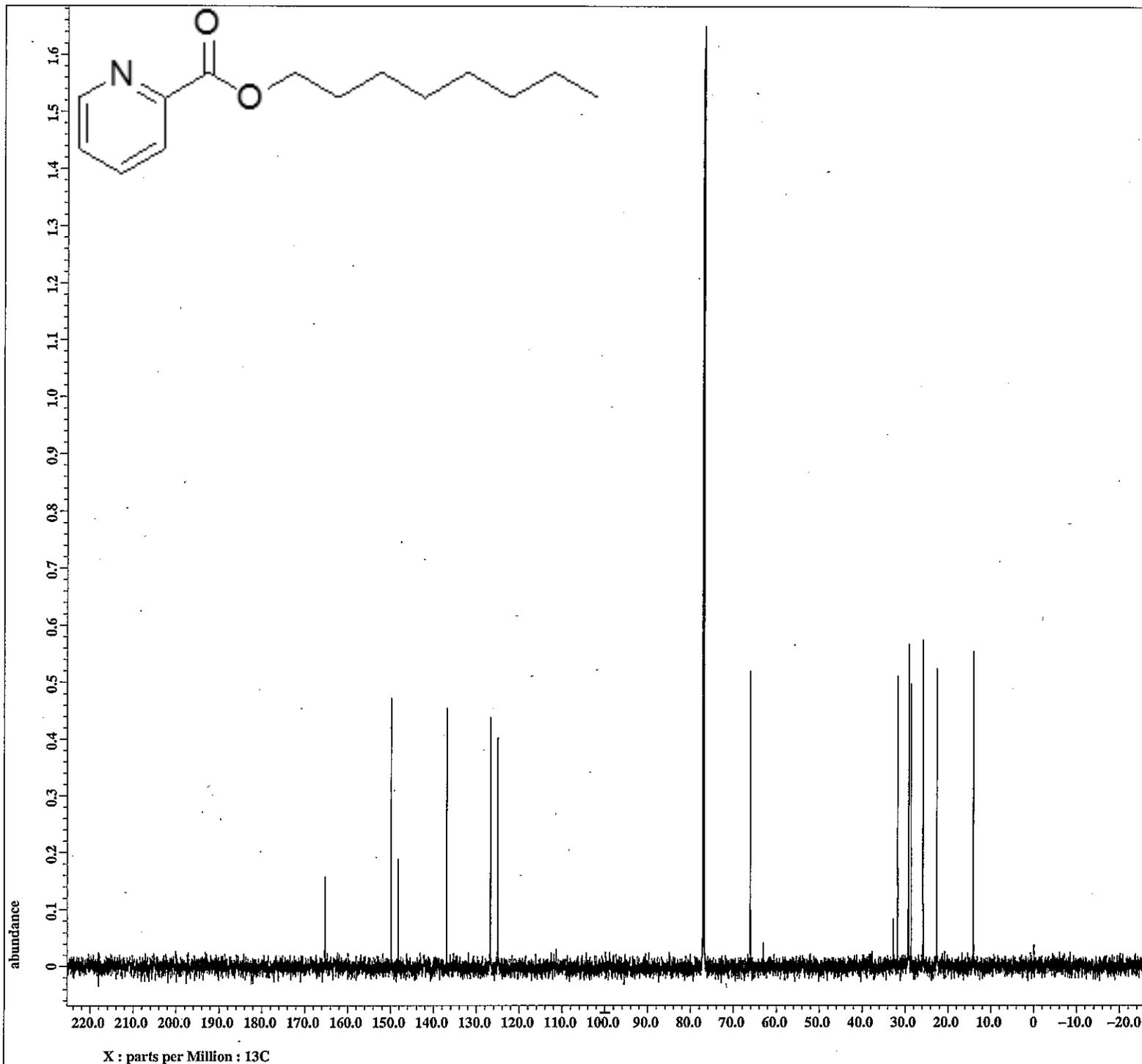


Filename = Exp-T-3-7-proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-T-3-7-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:08:51  
Revision\_time = 5-DEC-2012 20:32:44  
Current\_time = 5-DEC-2012 20:32:52

Content = Exp-T-3-7-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 = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 44  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.2[°C]

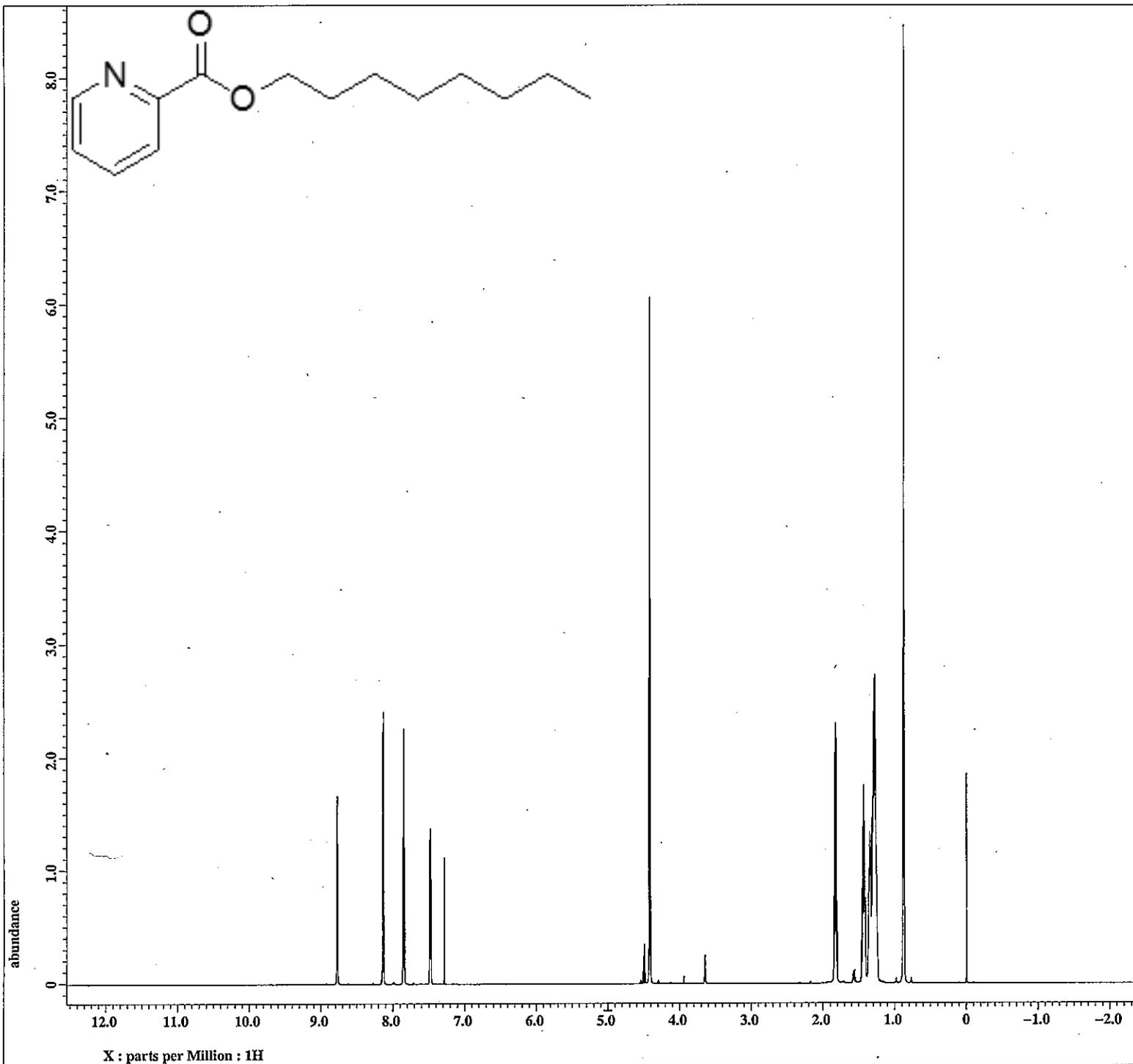


Filename = Exp-T-3-7-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-3-7-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:14:02  
Revision\_time = 5-DEC-2012 20:33:19  
Current\_time = 5-DEC-2012 20:33:27

Content = Exp-T-3-7-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\_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 = 100  
Total\_scans = 100

X\_90\_width = 11.3 [us]  
X\_acq\_time = 0.69206016 [s]  
X\_angle = 30 [deg]  
X\_atn = 8 [dB]  
X\_pulse = 3.76666667 [us]  
Irr\_atn\_dec = 19.34784 [dB]  
Irr\_atn\_noe = 19.34784 [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 = 19.8 [dC]



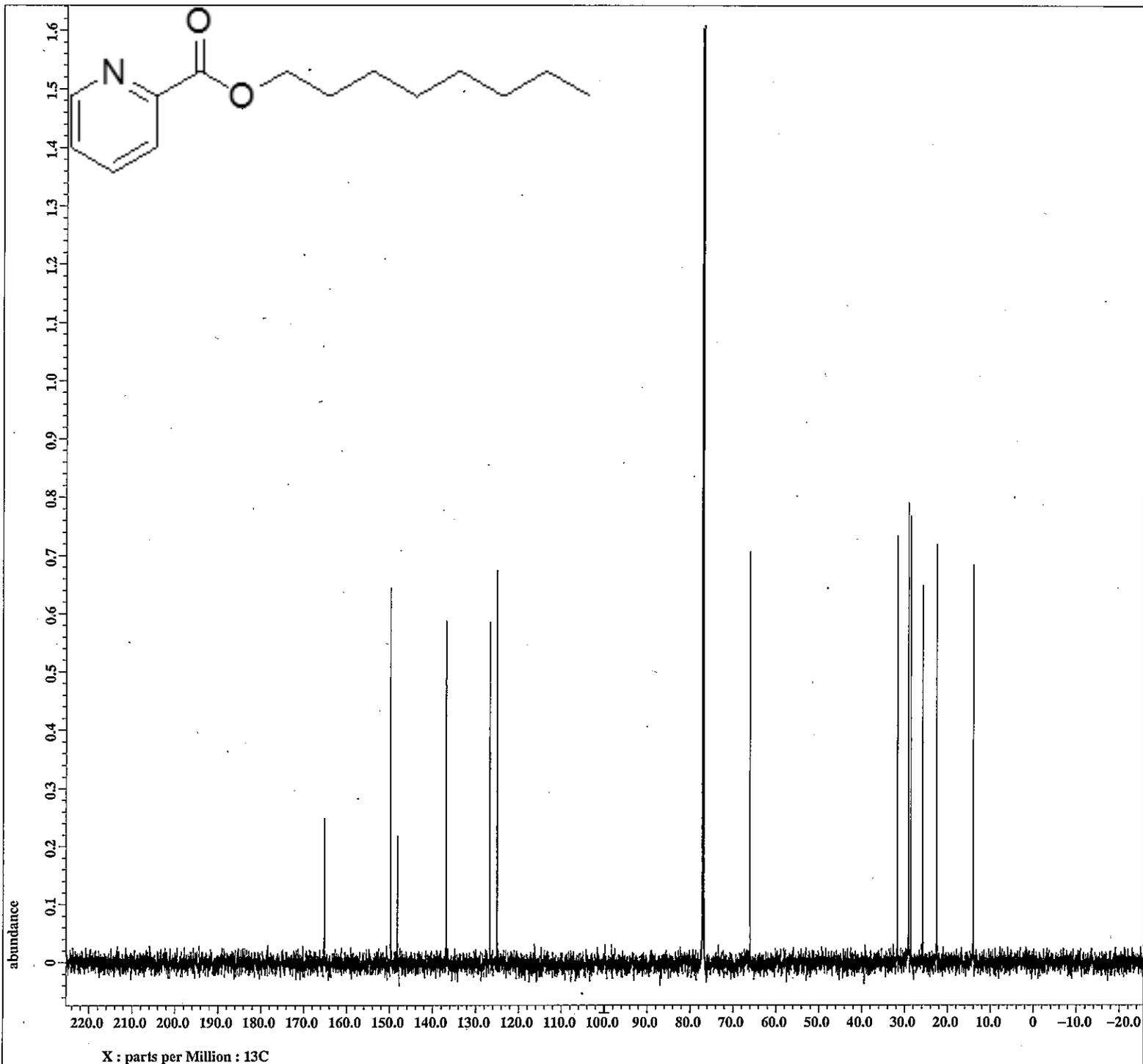
Filename = Exp-T-3-8-proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-T-3-8-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:22:40  
Revision\_time = 5-DEC-2012 20:36:15  
Current\_time = 5-DEC-2012 20:36:25

Content = Exp-T-3-8-proton  
Data\_format = 1D COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 42  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.1[degC]

X : parts per Million : 1H

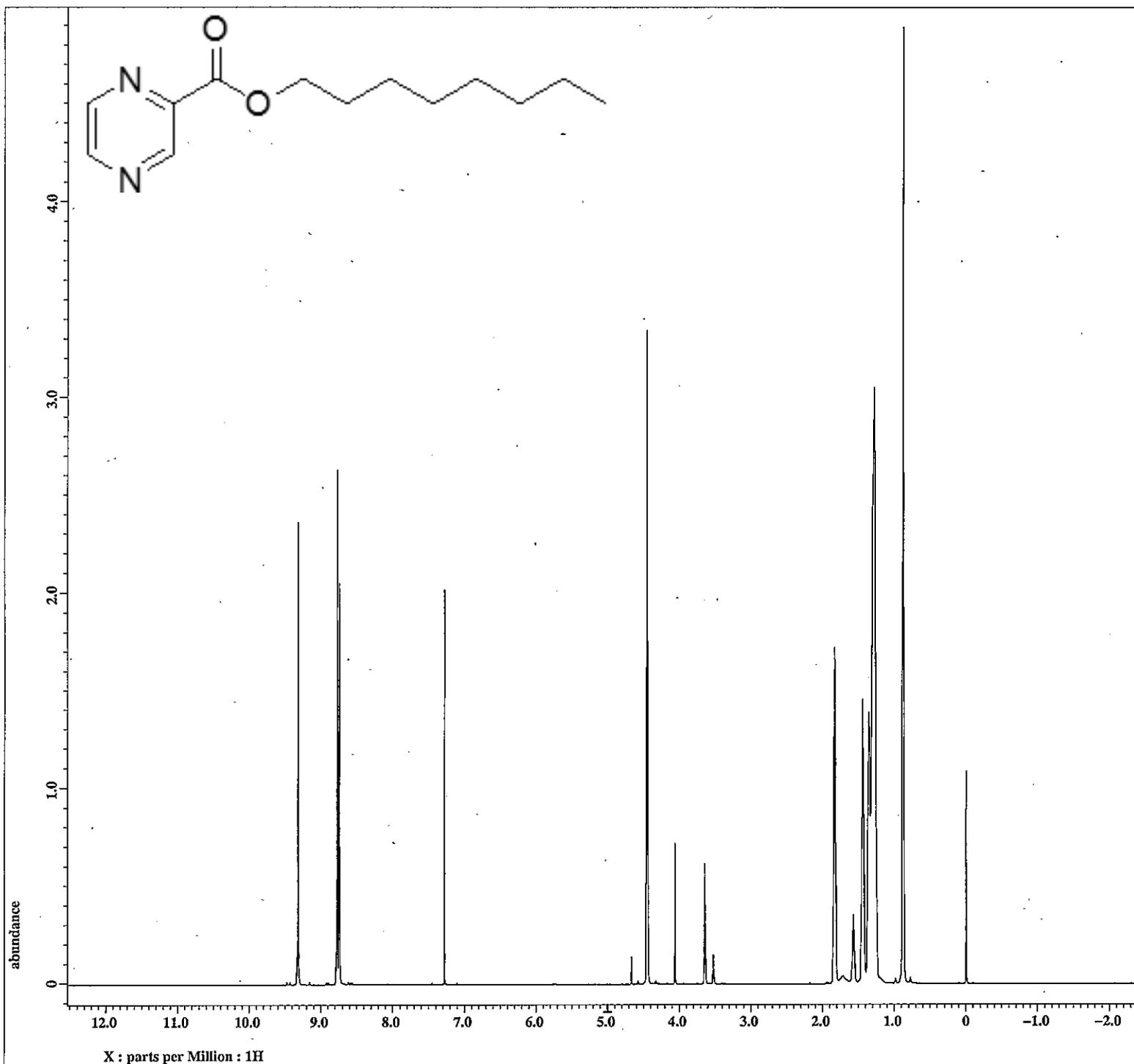
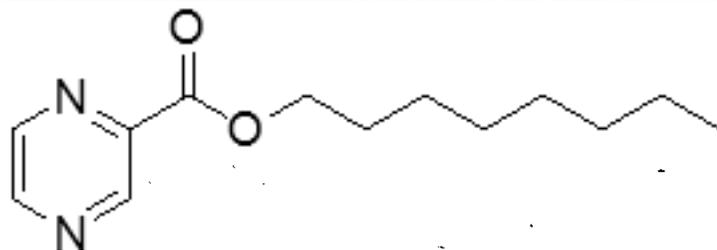


Filename = Exp-T-3-8-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-3-8-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:26:54  
Revision\_time = 5-DEC-2012 20:37:01  
Current\_time = 5-DEC-2012 20:37:09

Content = Exp-T-3-8-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 78  
Total\_scans = 78

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[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 = 19.9[dc]

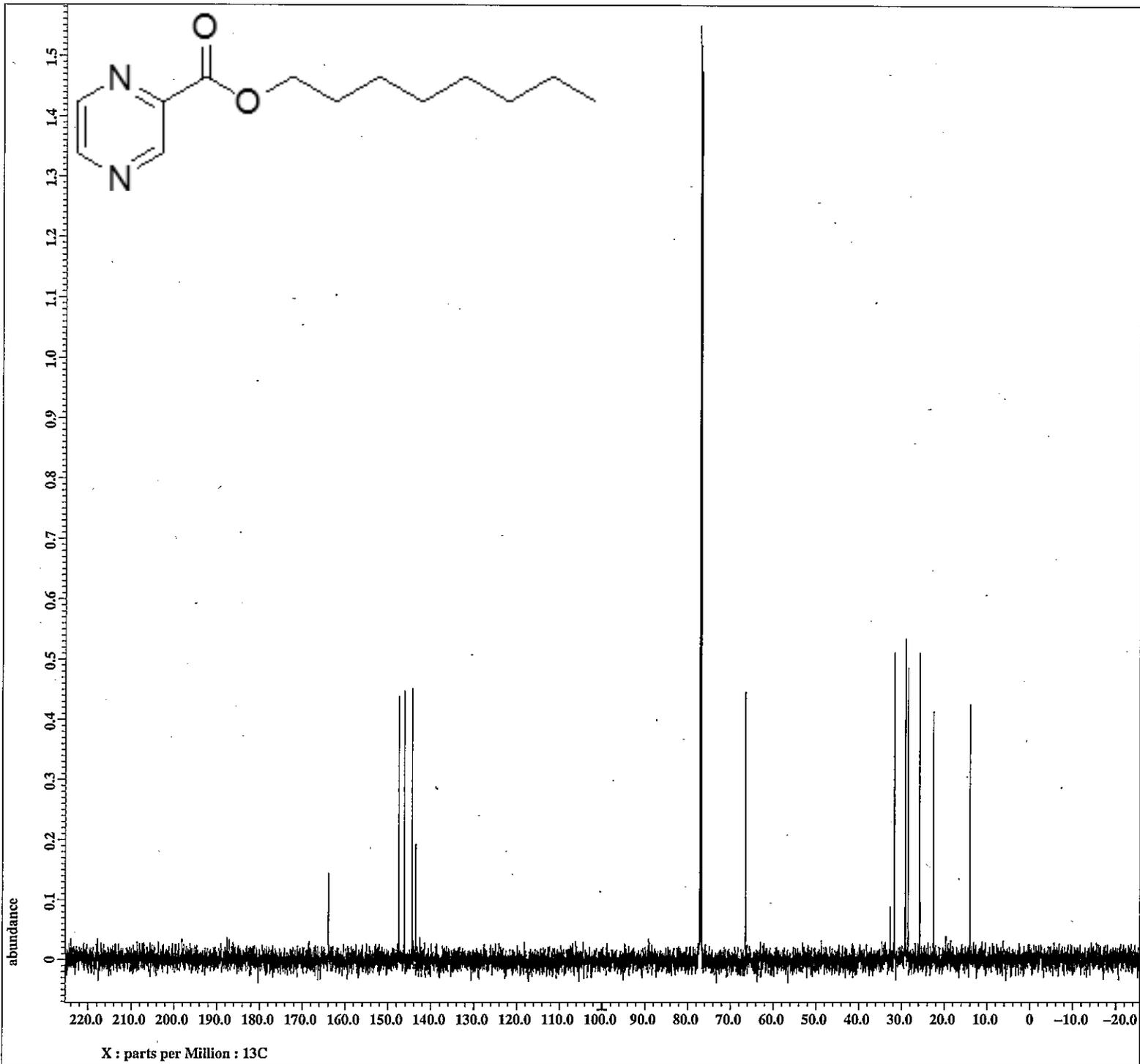


Filename = Exp-T-3-9-proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-T-3-9-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:32:40  
Revision\_time = 5-DEC-2012 20:37:47  
Current\_time = 5-DEC-2012 20:37:57

Content = Exp-T-3-9-proton  
Data\_format = 1D COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 44  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.6[dc]

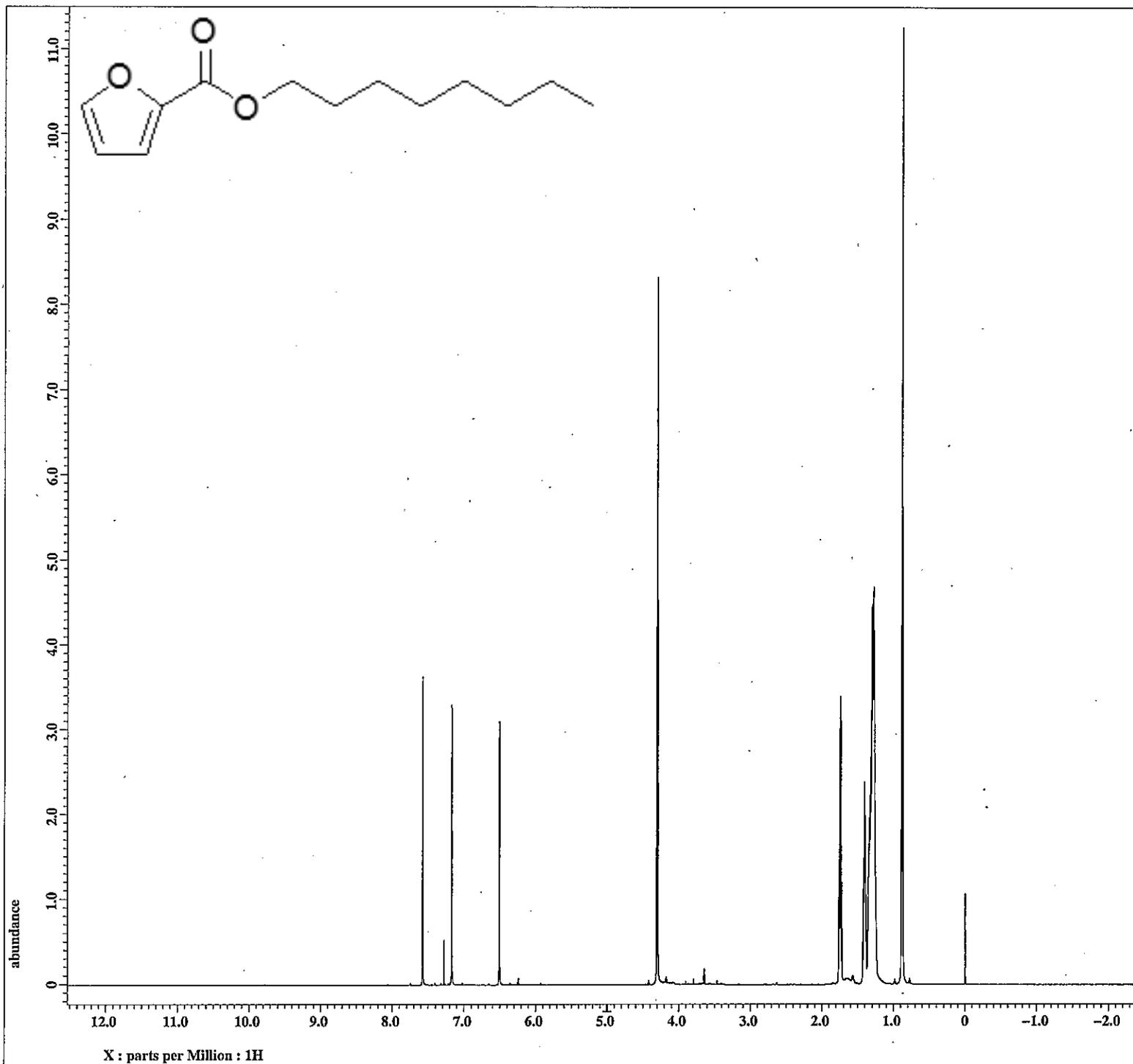


Filename = Exp-T-3-9-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-3-9-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:36:23  
Revision\_time = 5-DEC-2012 20:38:32  
Current\_time = 5-DEC-2012 20:38:38

Content = Exp-T-3-9-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 67  
Total\_scans = 67

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[dB]  
Irr\_noise = WALTZ  
Decoupling = TRUE  
Initial\_wait = 1[s]  
Noe = TRUE  
Noe\_time = 2[s]  
Recvr\_gain = 60  
Relaxation\_delay = 2[s]  
Repetition\_time = 2.69206016[s]  
Temp\_get = 20.1[dc]

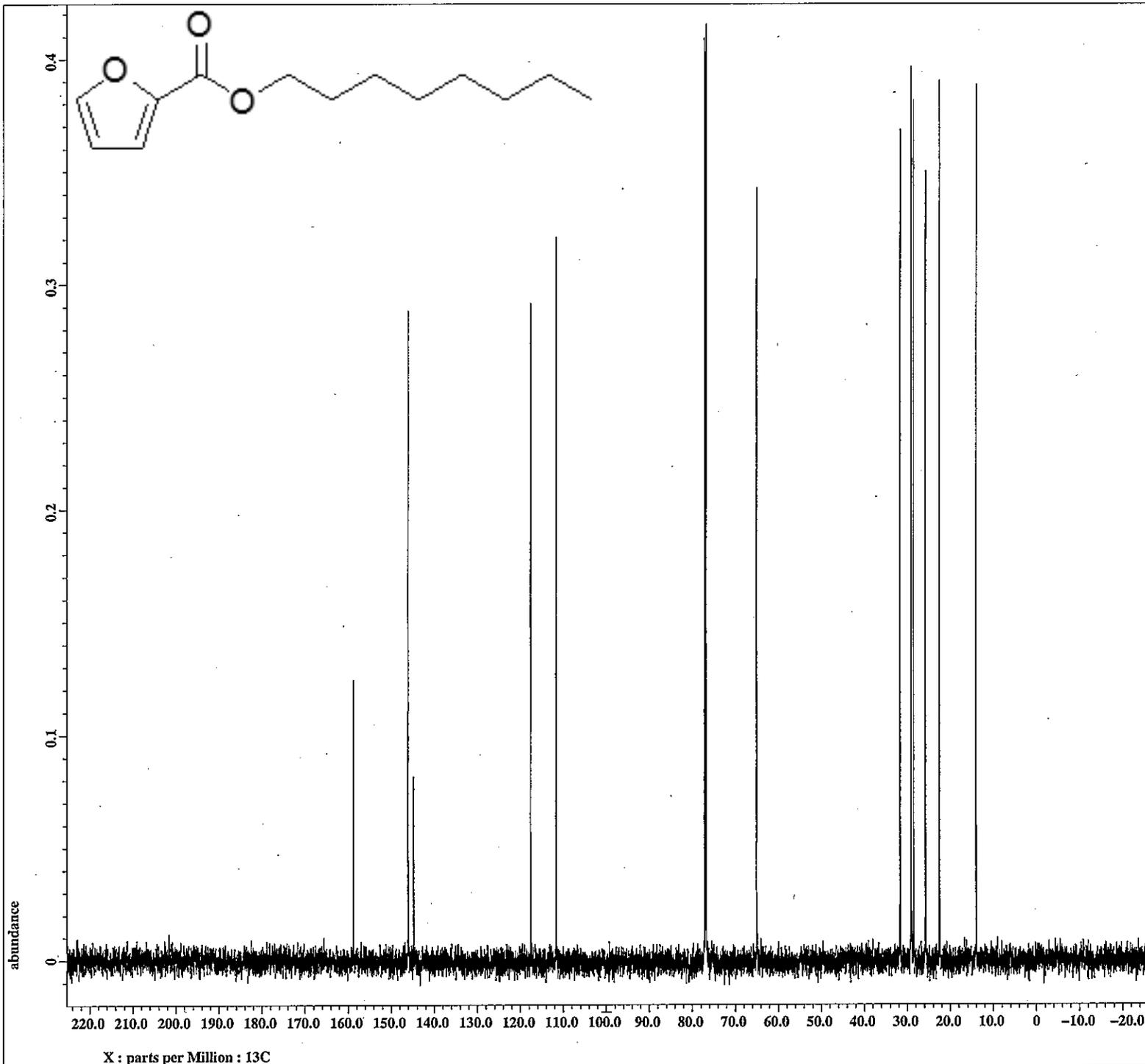


Filename = Exp-T-3-10-proton-3.j  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-T-3-10-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:42:24  
Revision\_time = 5-DEC-2012 20:39:39  
Current\_time = 5-DEC-2012 20:39:46

Content = Exp-T-3-10-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 = TRUE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 40  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.3[dc]

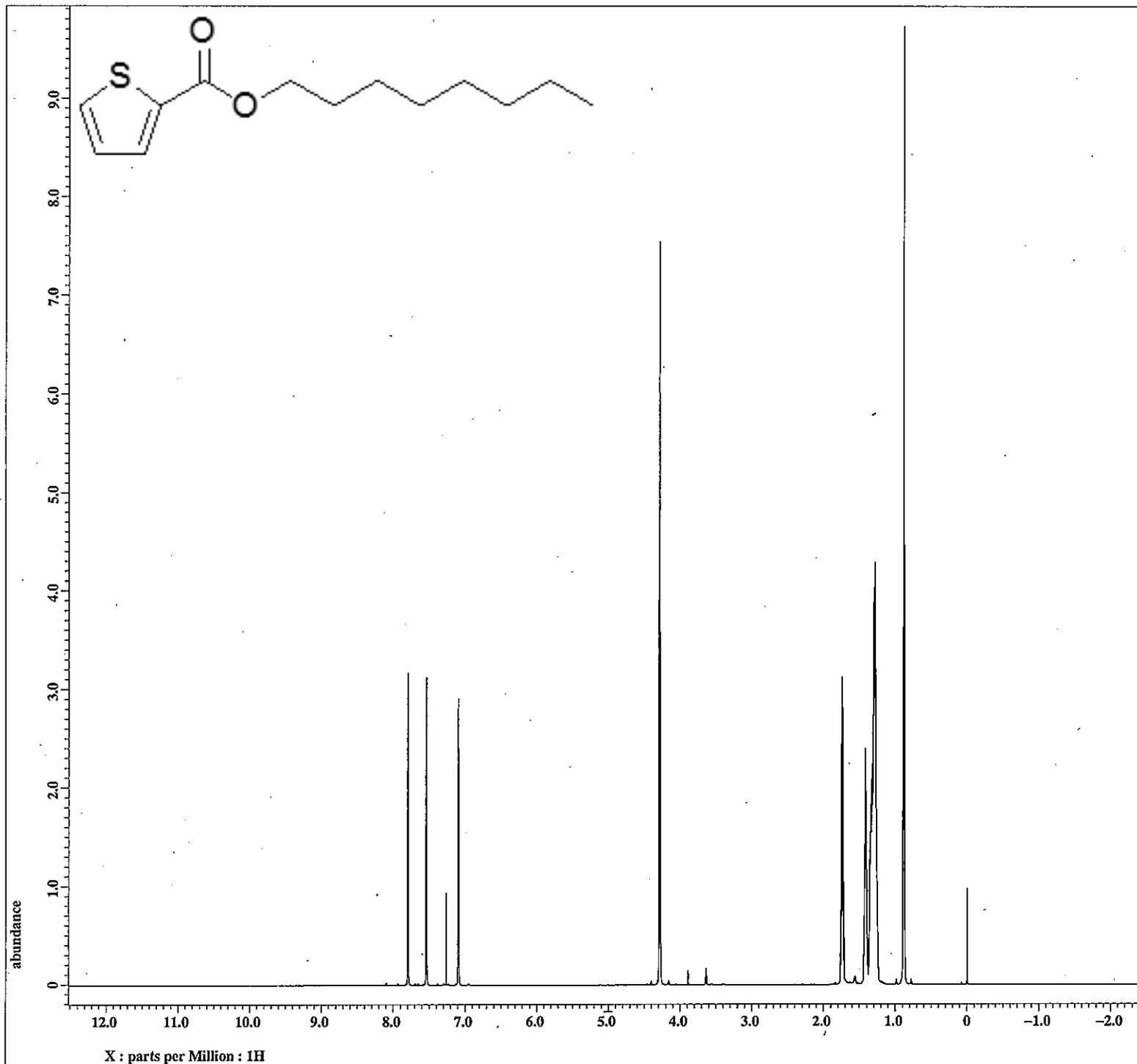


Filename = Exp-T-3-10-carbon-3.j  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-3-10-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:46:04  
Revision\_time = 5-DEC-2012 21:37:25  
Current\_time = 5-DEC-2012 21:37:32

Content = Exp-T-3-10-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 76  
Total\_scans = 76

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[dB]  
Irr\_noise = WALTZ  
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 = 20[dc]

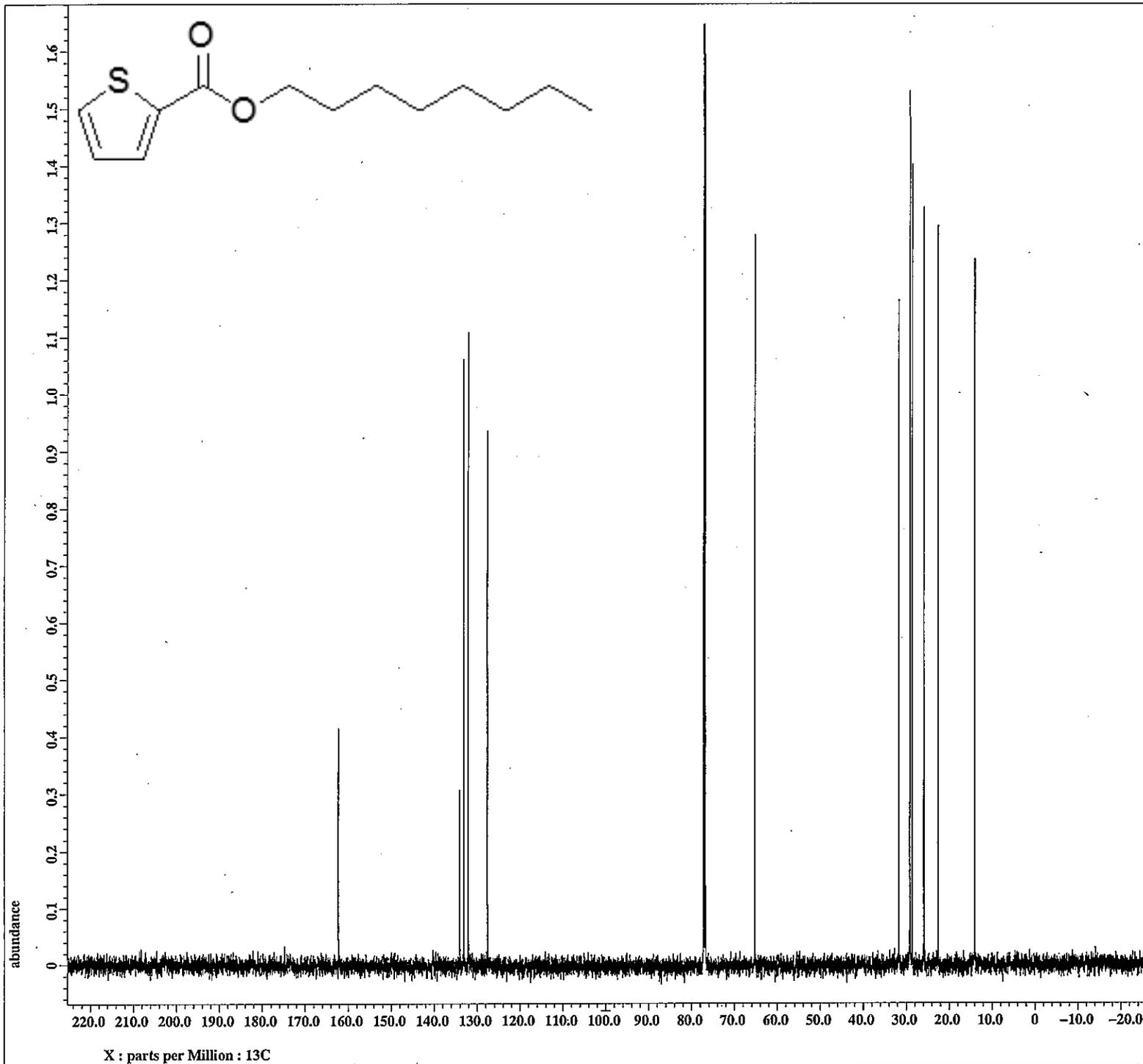


Filename = Exp-T-3-11-proton-3.j  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-T-3-11-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:52:11  
Revision\_time = 5-DEC-2012 20:41:51  
Current\_time = 5-DEC-2012 20:41:57

Content = Exp-T-3-11-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 = TRUE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 40  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19[dC]

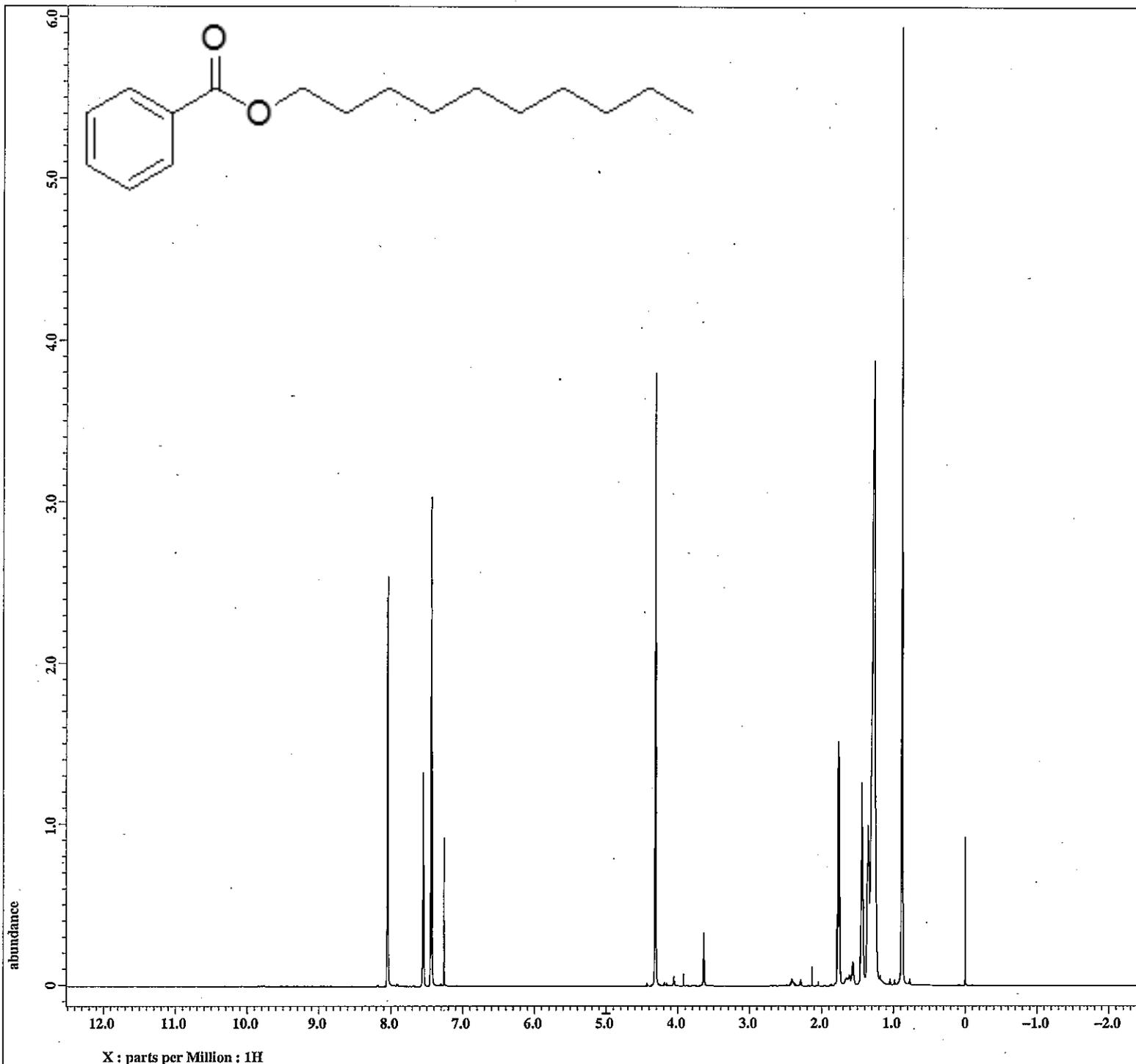
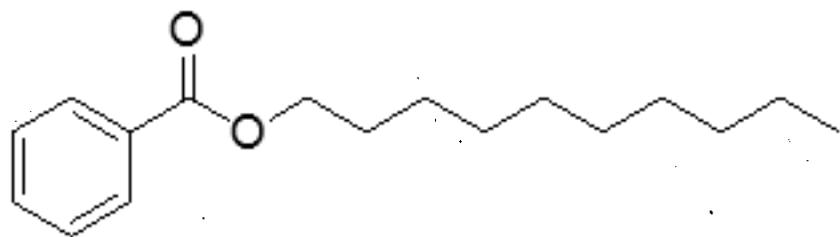


Filename = Exp-T-3-11-carbon-3.j  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-3-11-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 29-NOV-2012 21:57:29  
Revision\_time = 5-DEC-2012 20:42:32  
Current\_time = 5-DEC-2012 20:42:38

Content = Exp-T-3-11-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 102  
Total\_scans = 102

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[db]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[db]  
Irr\_atn\_noe = 19.34784[db]  
Irr\_noise = WALTZ  
Decoupling = TRUE  
Initial\_wait = 1[s]  
Noe = TRUE  
Noe\_time = 2[s]  
Recvr\_gain = 60  
Relaxation\_delay = 2[s]  
Repetition\_time = 2.69206016[s]  
Temp\_get = 20.1[dc]

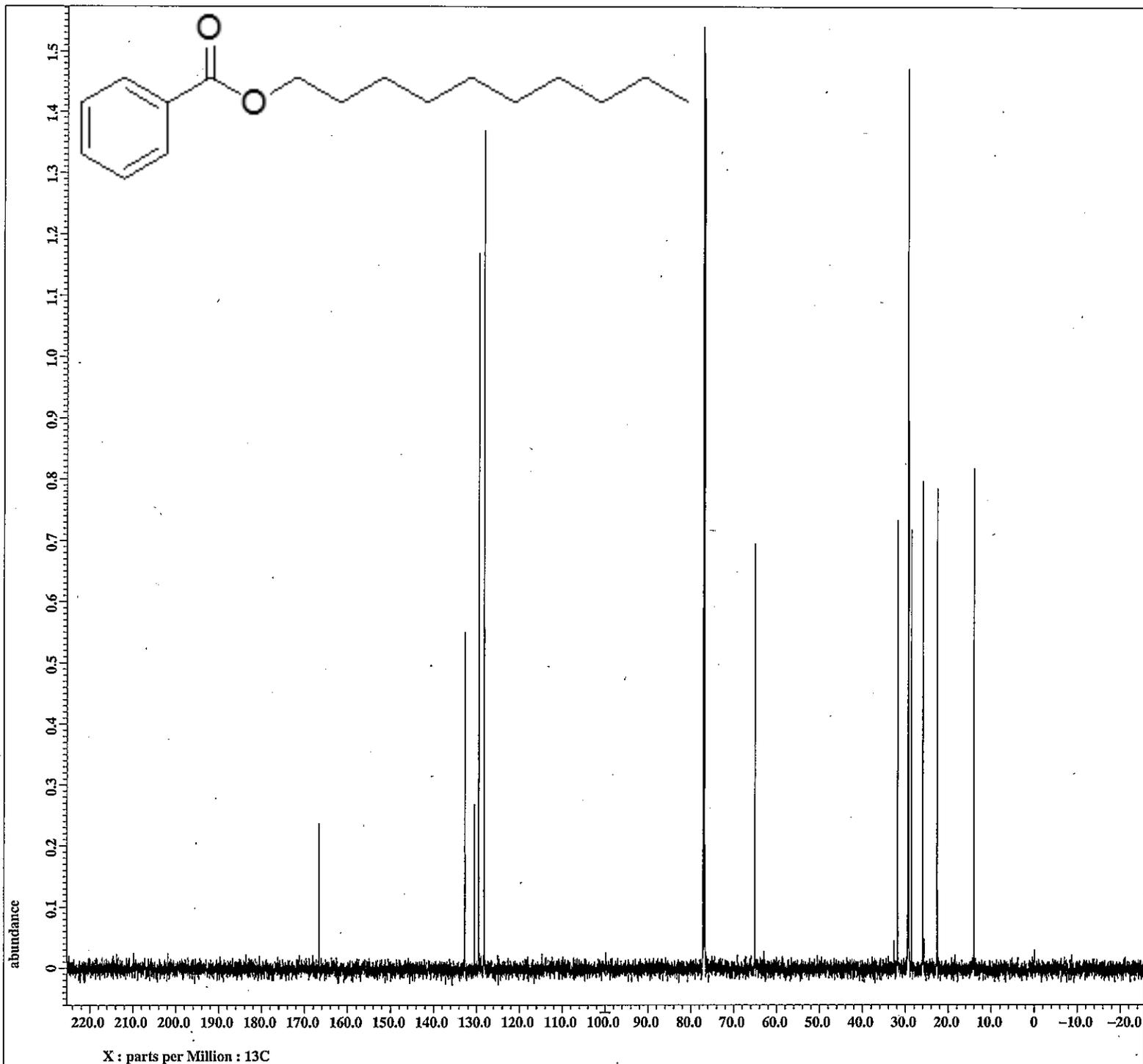


Filename = EXP-T-4-2-Proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = EXP-T-4-2-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 19:15:32  
Revision\_time = 5-DEC-2012 20:43:24  
Current\_time = 5-DEC-2012 20:43:32

Content = EXP-T-4-2-Proton  
Data\_format = 1D\_COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 38  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 18.9[dC]

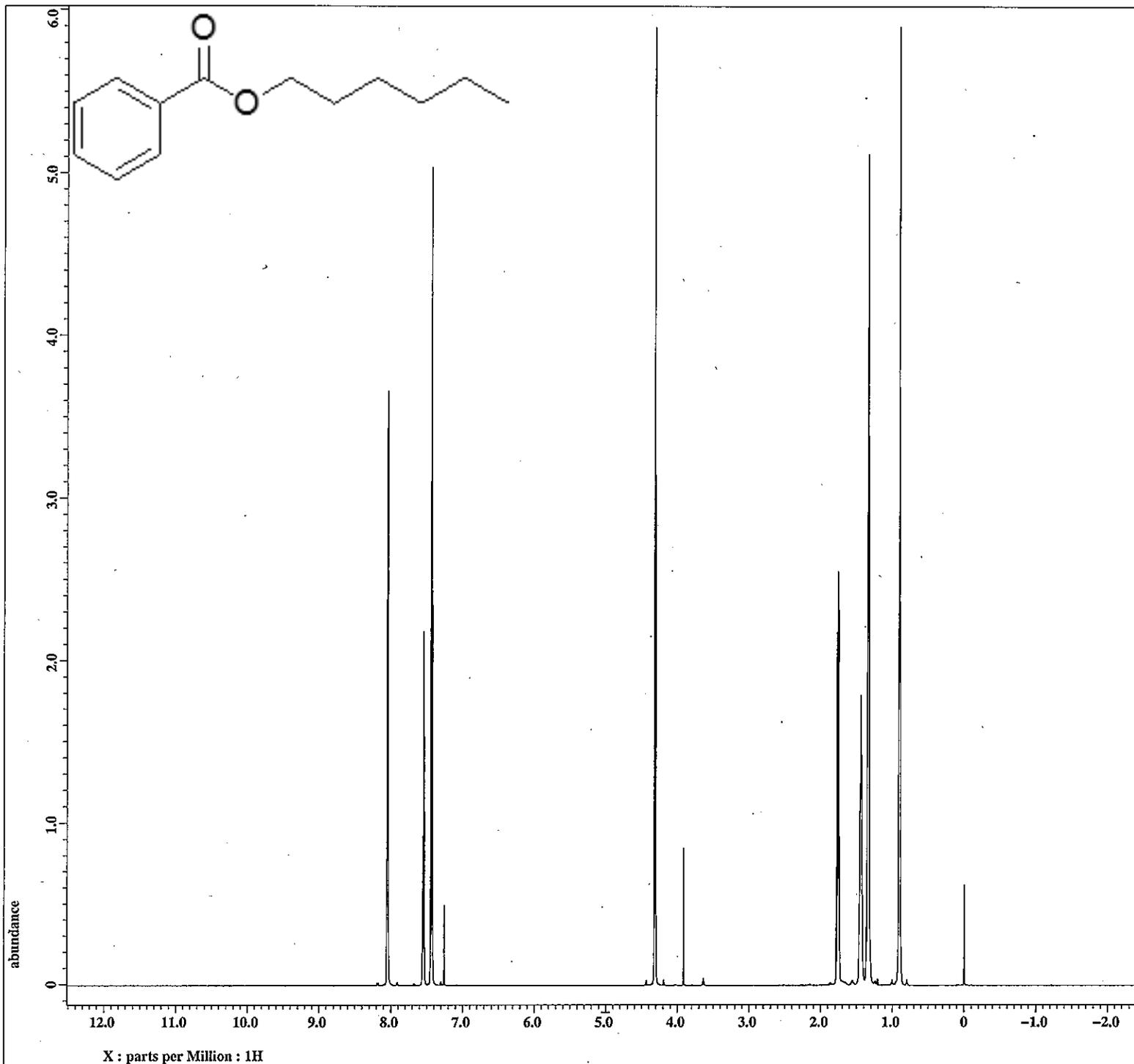


Filename = Exp-T-4-2-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-2-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 19:22:16  
Revision\_time = 5-DEC-2012 20:44:09  
Current\_time = 5-DEC-2012 20:44:18

Content = Exp-T-4-2-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 134  
Total\_scans = 134

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[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 = 19.7[degC]

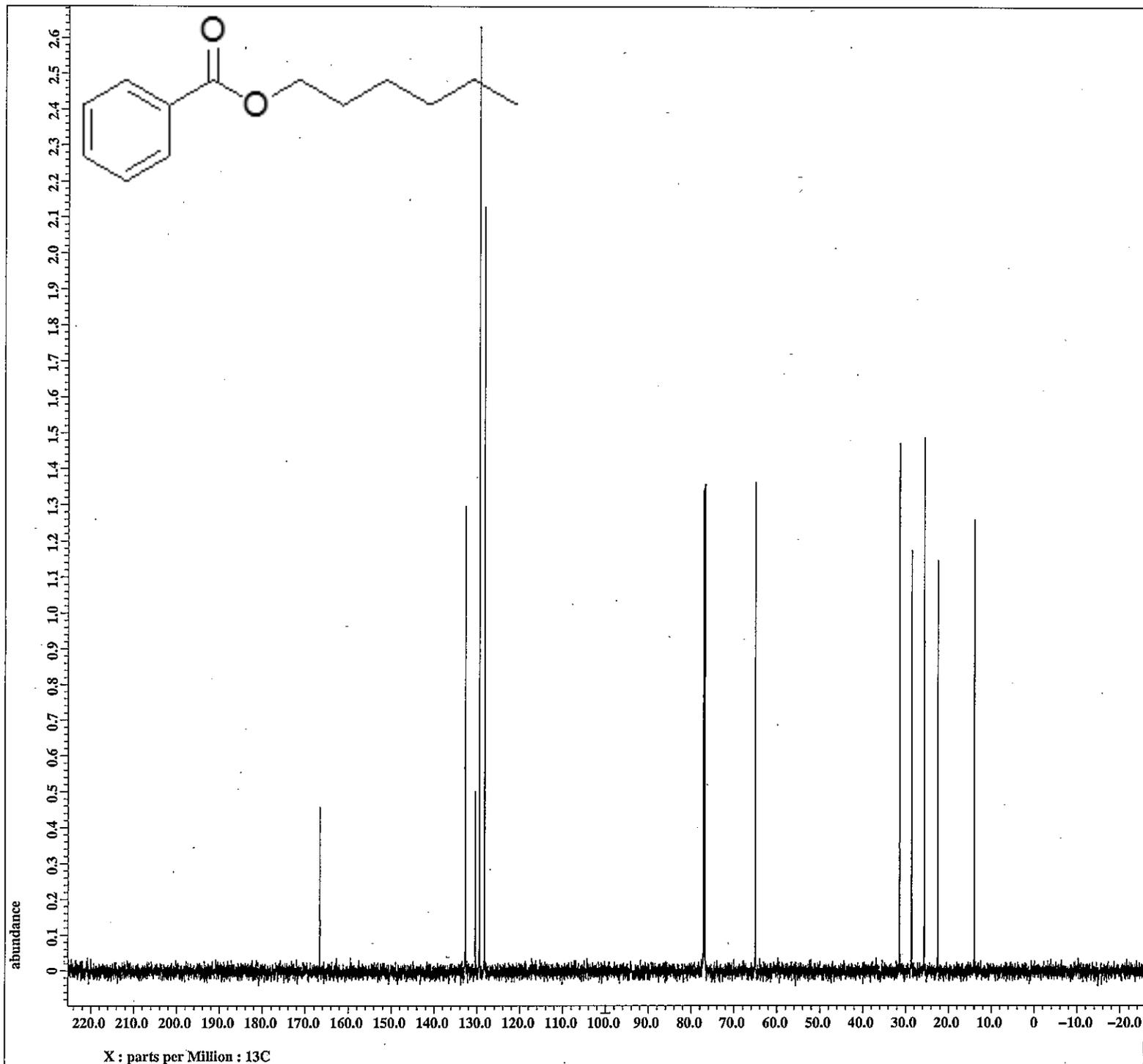


Filename = EXP-T-4-3-Proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = EXP-T-4-3-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 19:27:56  
Revision\_time = 5-DEC-2012 20:46:47  
Current\_time = 5-DEC-2012 20:46:54

Content = EXP-T-4-3-Proton  
Data\_format = 1D COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[db]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 36  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19[dC]

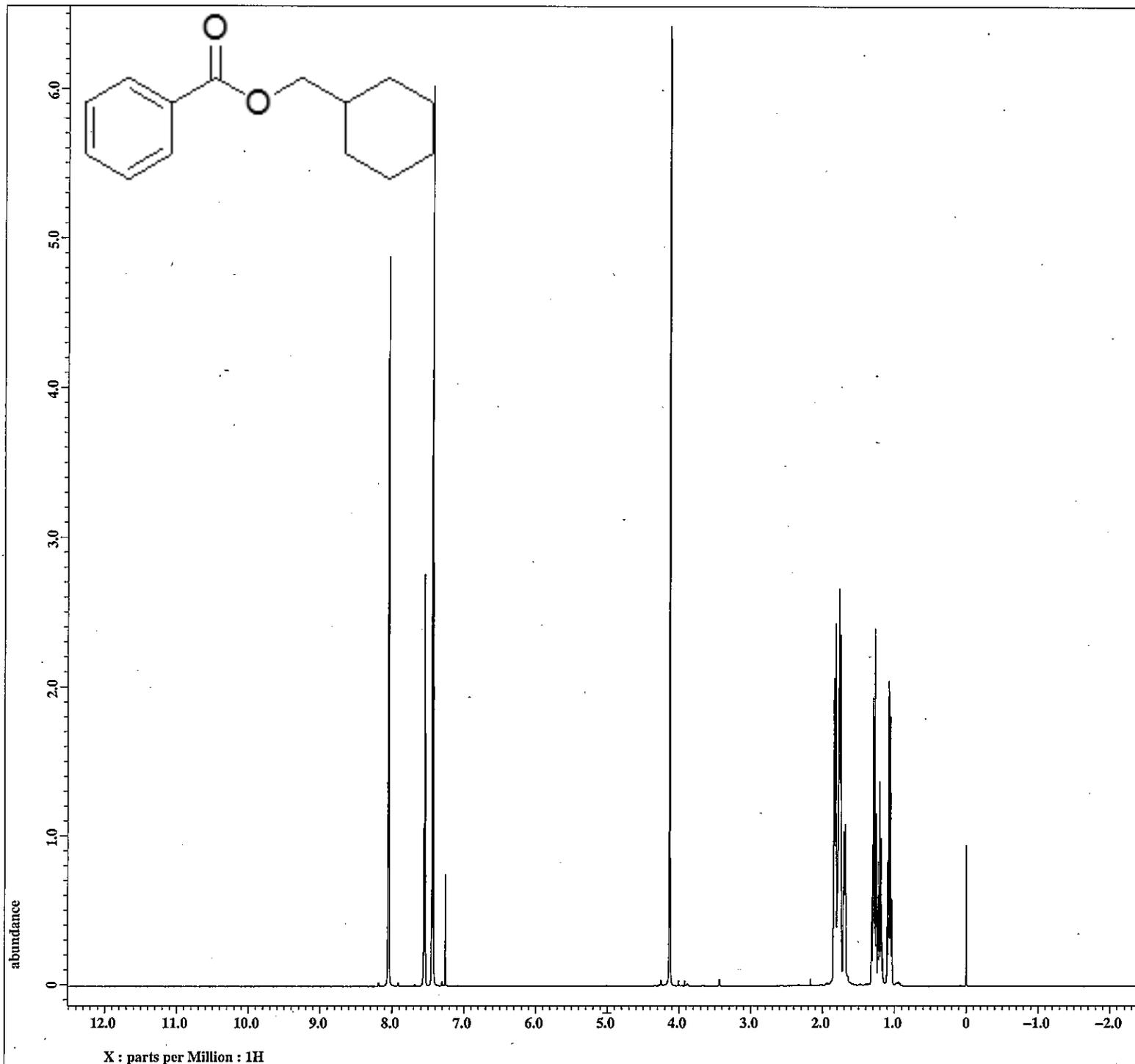


Filename = Exp-T-4-3-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-3-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 19:31:12  
Revision\_time = 5-DEC-2012 20:46:00  
Current\_time = 5-DEC-2012 20:46:08

Content = Exp-T-4-3-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 57  
Total\_scans = 57

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[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 = 19.5[degC]

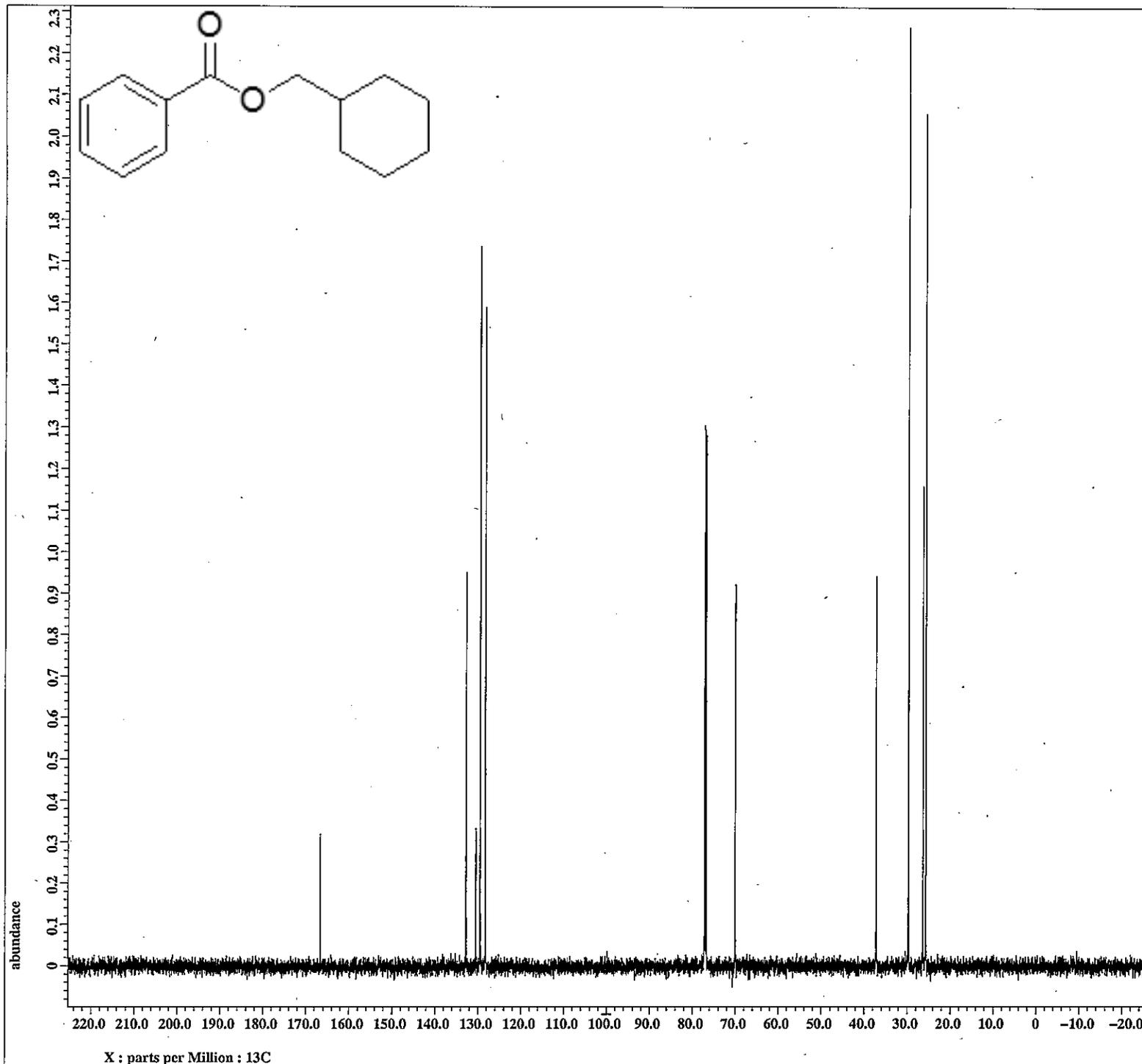


Filename = EXP-T-4-5-Proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = EXP-T-4-5-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 19:52:39  
Revision\_time = 5-DEC-2012 20:47:49  
Current\_time = 5-DEC-2012 20:47:55

Content = EXP-T-4-5-Proton  
Data\_format = 1D COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_preset = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 40  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 18.9[dC]

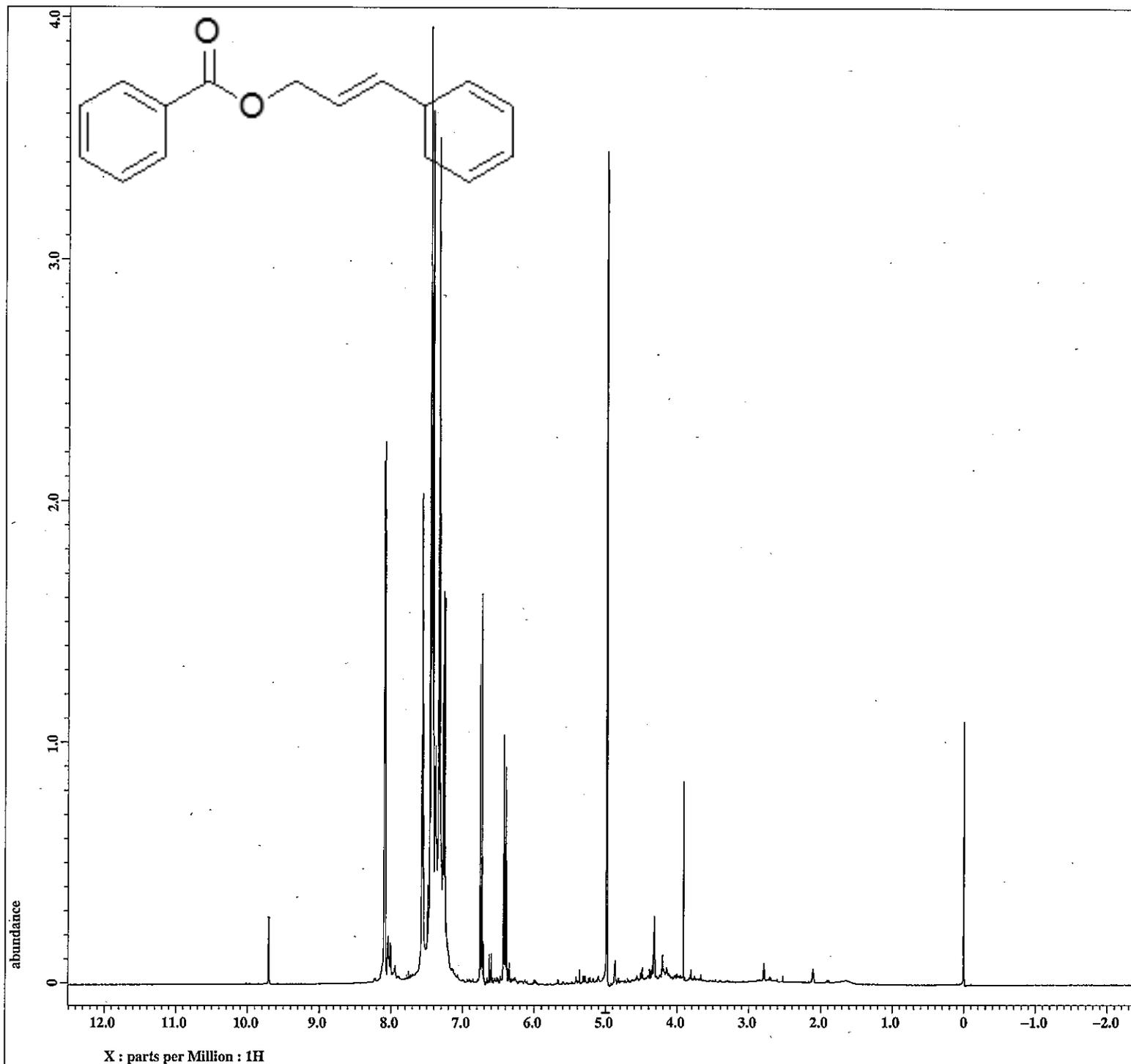


Filename = Exp-T-4-5-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-5-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 19:56:42  
Revision\_time = 5-DEC-2012 20:48:41  
Current\_time = 5-DEC-2012 20:48:49

Content = Exp-T-4-5-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA-600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928 [T] (600[M]  
X\_acq\_duration = 0.69206016 [s]  
X\_domain = 13C  
X\_freq = 150.91343039 [MHz]  
X\_offset = 100 [ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109 [Hz]  
X\_sweep = 47.34848485 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 74  
Total\_scans = 74

X\_90\_width = 11.3 [us]  
X\_acq\_time = 0.69206016 [s]  
X\_angle = 30 [deg]  
X\_atn = 8 [dB]  
X\_pulse = 3.76666667 [us]  
Irr\_atn\_dec = 19.34784 [dB]  
Irr\_atn\_noe = 19.34784 [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 = 19.8 [dC]

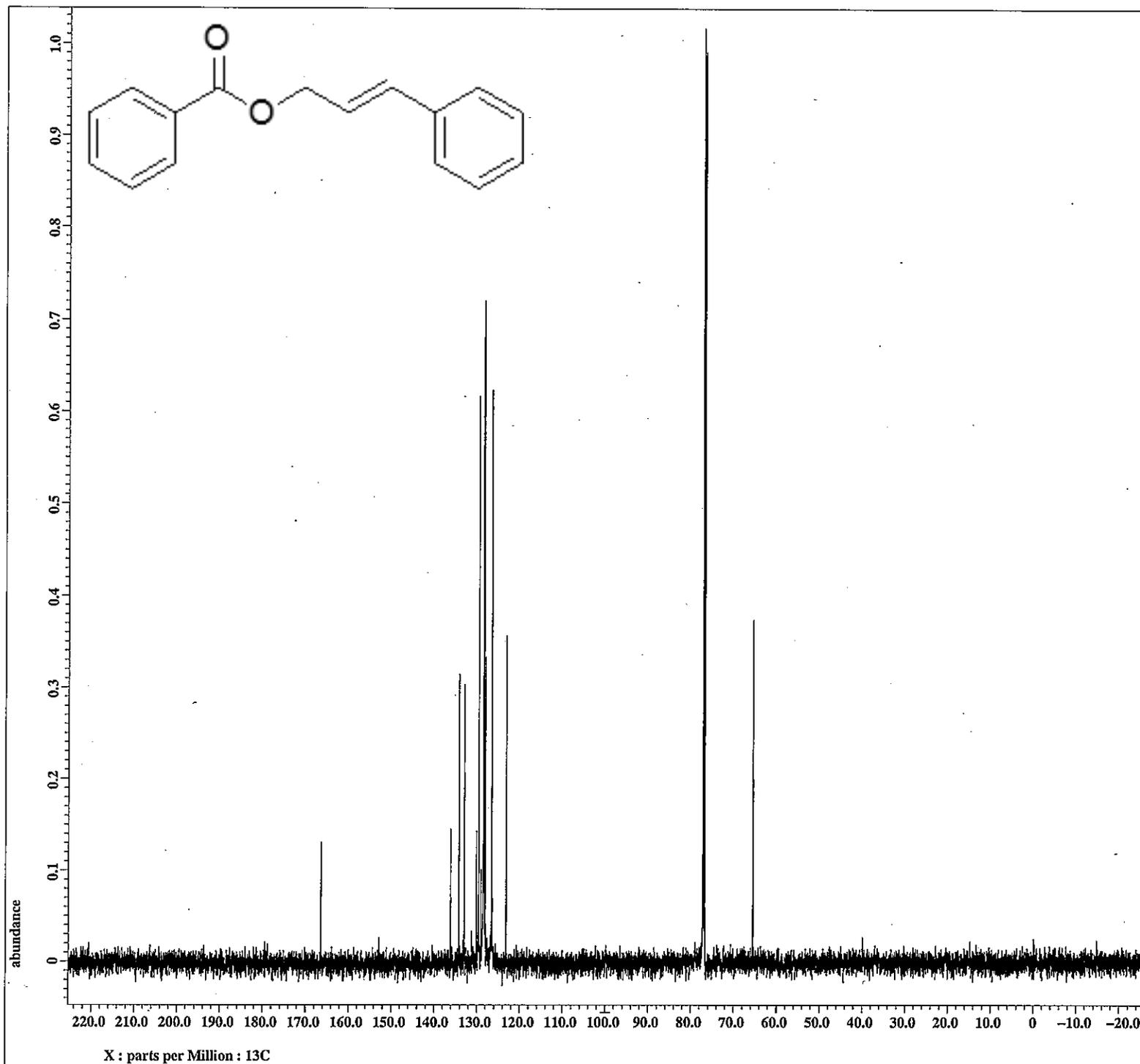


Filename = EXP-T-4-6-Proton-2.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = EXP-T-4-6-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 19:37:35  
Revision\_time = 5-DEC-2012 20:50:07  
Current\_time = 5-DEC-2012 20:50:20

Content = EXP-T-4-6-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 = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 44  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 18.9[dC]

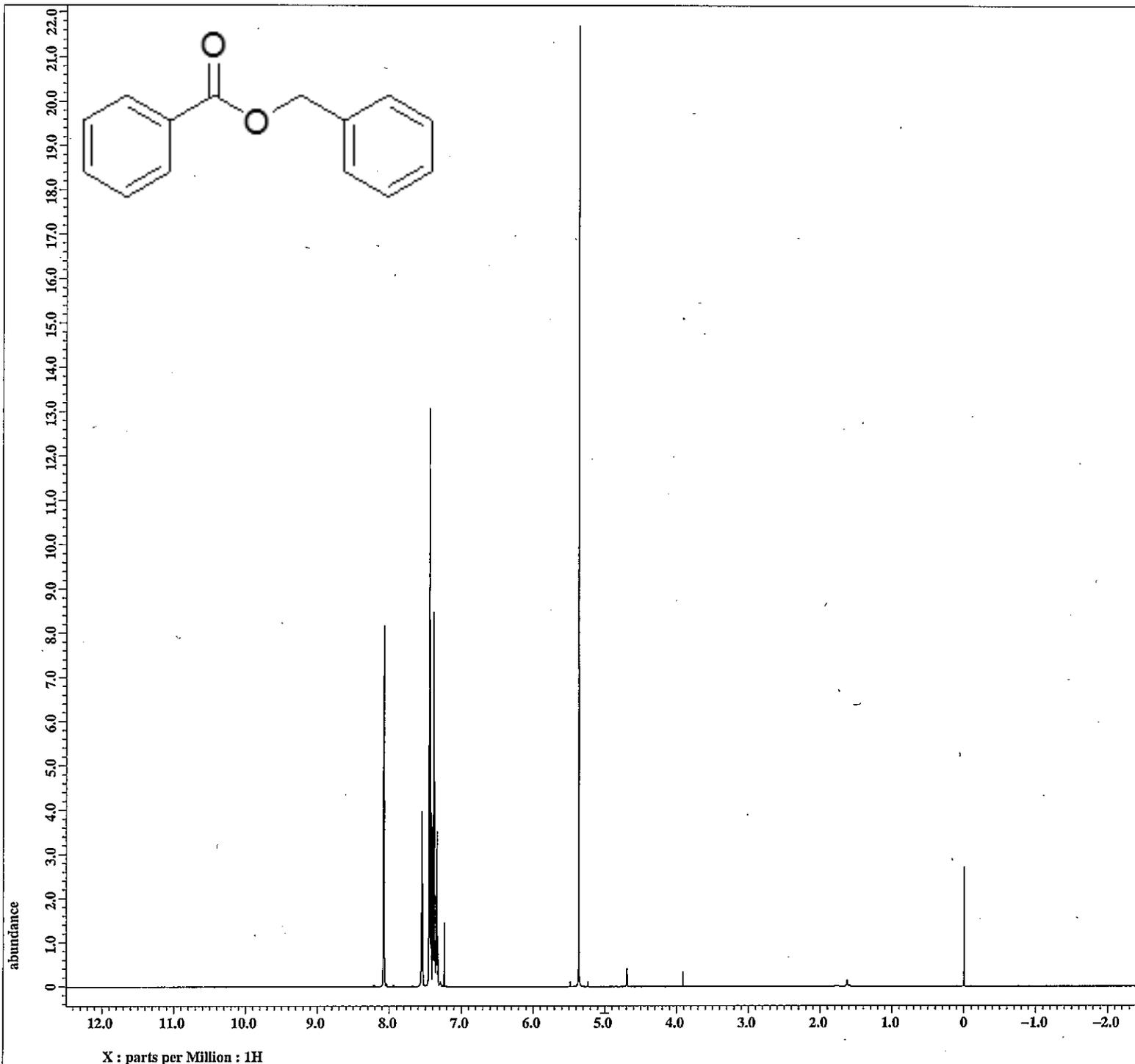
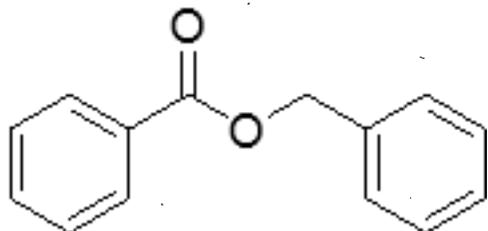


Filename = Exp-T-4-6-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-6-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 19:45:20  
Revision\_time = 5-DEC-2012 20:51:03  
Current\_time = 5-DEC-2012 20:51:07

Content = Exp-T-4-6-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928 [T] (600 [M])  
X\_acq\_duration = 0.69206016 [s]  
X\_domain = 13C  
X\_freq = 150.91343039 [MHz]  
X\_offset = 100 [ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109 [Hz]  
X\_sweep = 47.34848485 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Clipped = TRUE  
Mod\_return = 1  
Scans = 157  
Total\_scans = 157

X\_90\_width = 11.3 [us]  
X\_acq\_time = 0.69206016 [s]  
X\_angle = 30 [deg]  
X\_atn = 8 [dB]  
X\_pulse = 3.76666667 [us]  
Irr\_atn\_dec = 19.34784 [dB]  
Irr\_atn\_noe = 19.34784 [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 = 19.8 [dC]

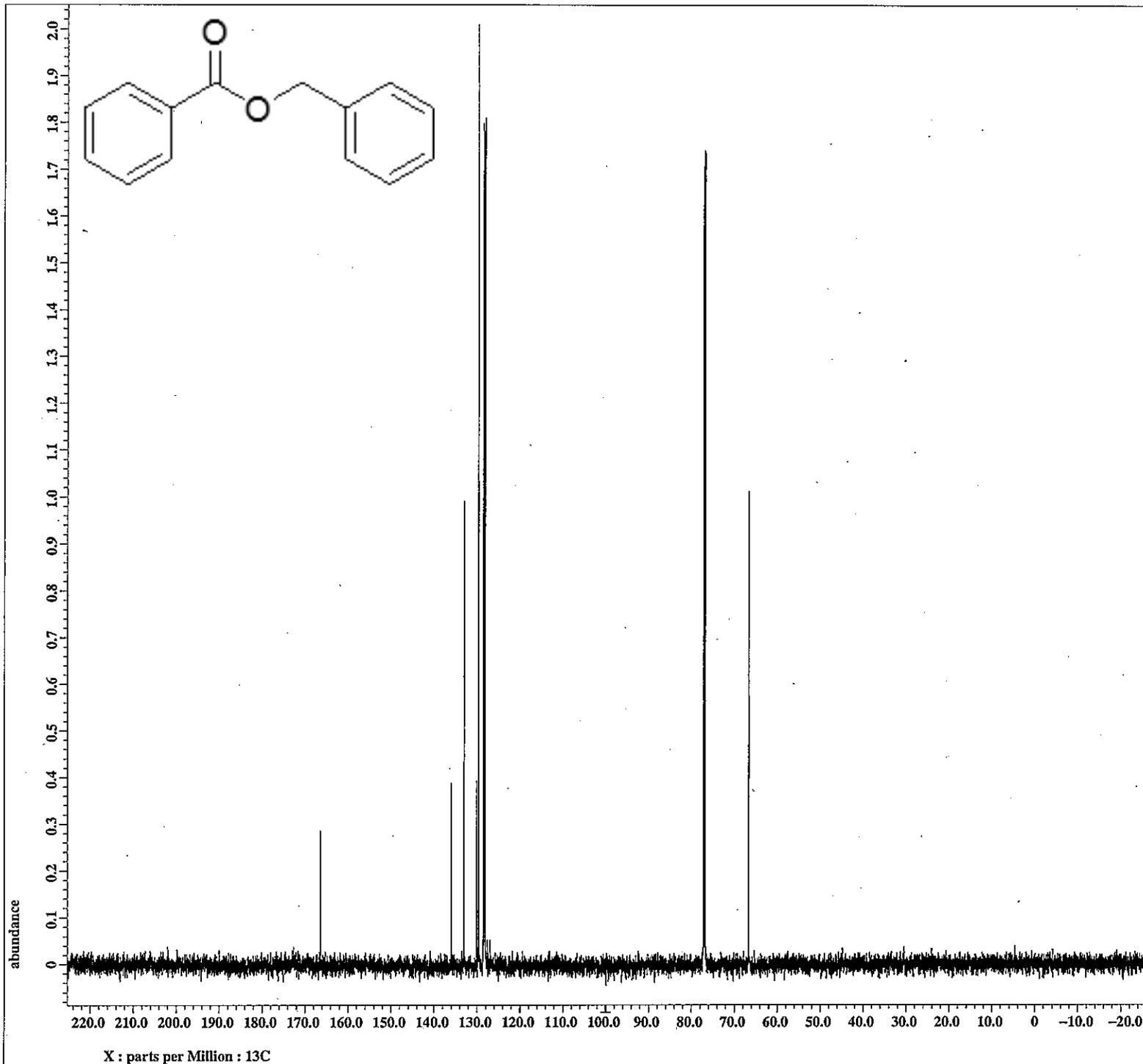


Filename = EXP-T-4-7-Proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = EXP-T-4-7-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:02:31  
Revision\_time = 5-DEC-2012 20:53:26  
Current\_time = 5-DEC-2012 20:53:34

Content = EXP-T-4-7-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 = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_preset = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 44  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.4[degC]

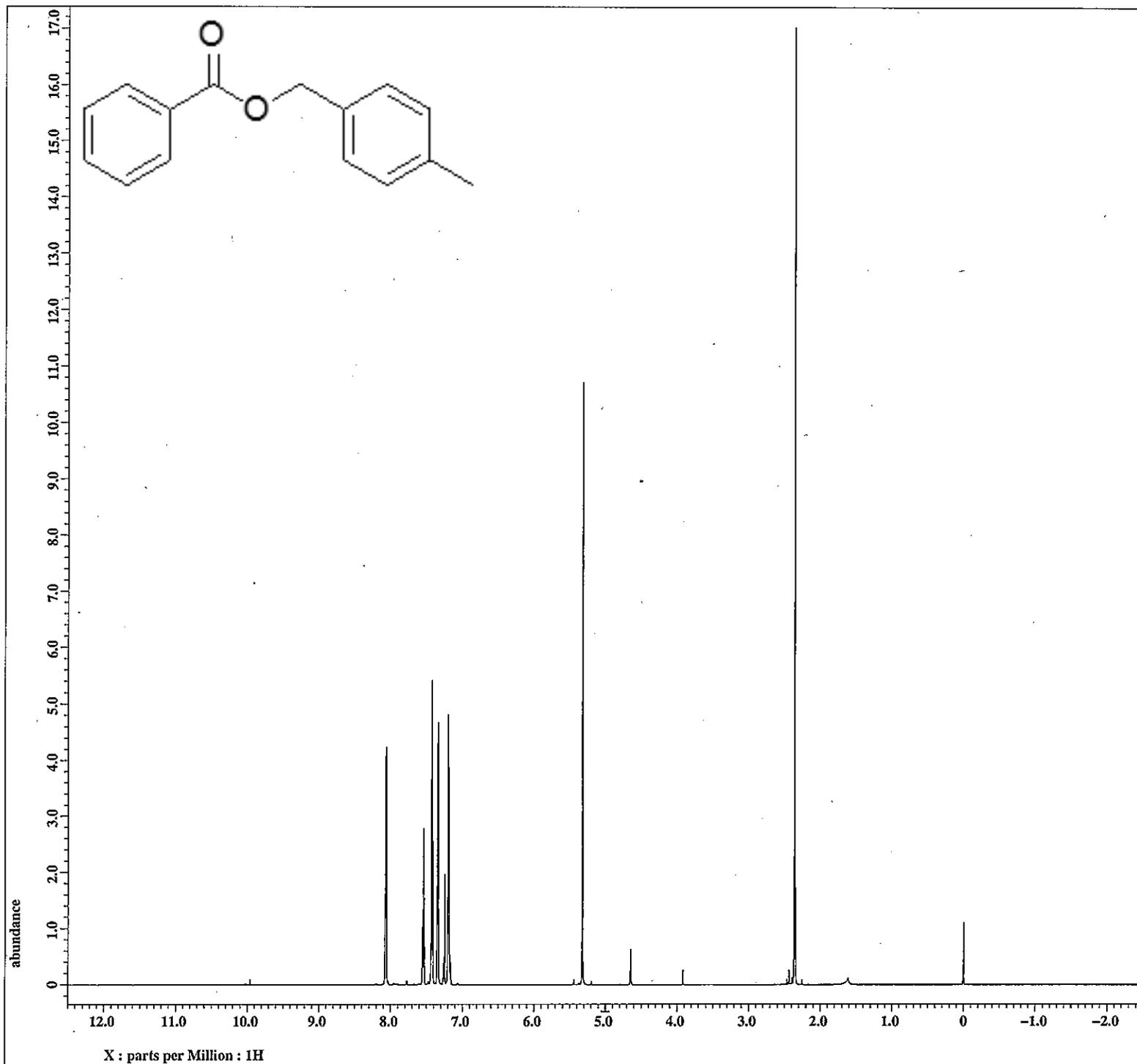


Filename = Exp-T-4-7-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-7-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:06:08  
Revision\_time = 5-DEC-2012 20:54:28  
Current\_time = 5-DEC-2012 20:54:33

Content = Exp-T-4-7-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\_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 = 65  
Total\_scans = 65

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[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 = 19.4[degC]

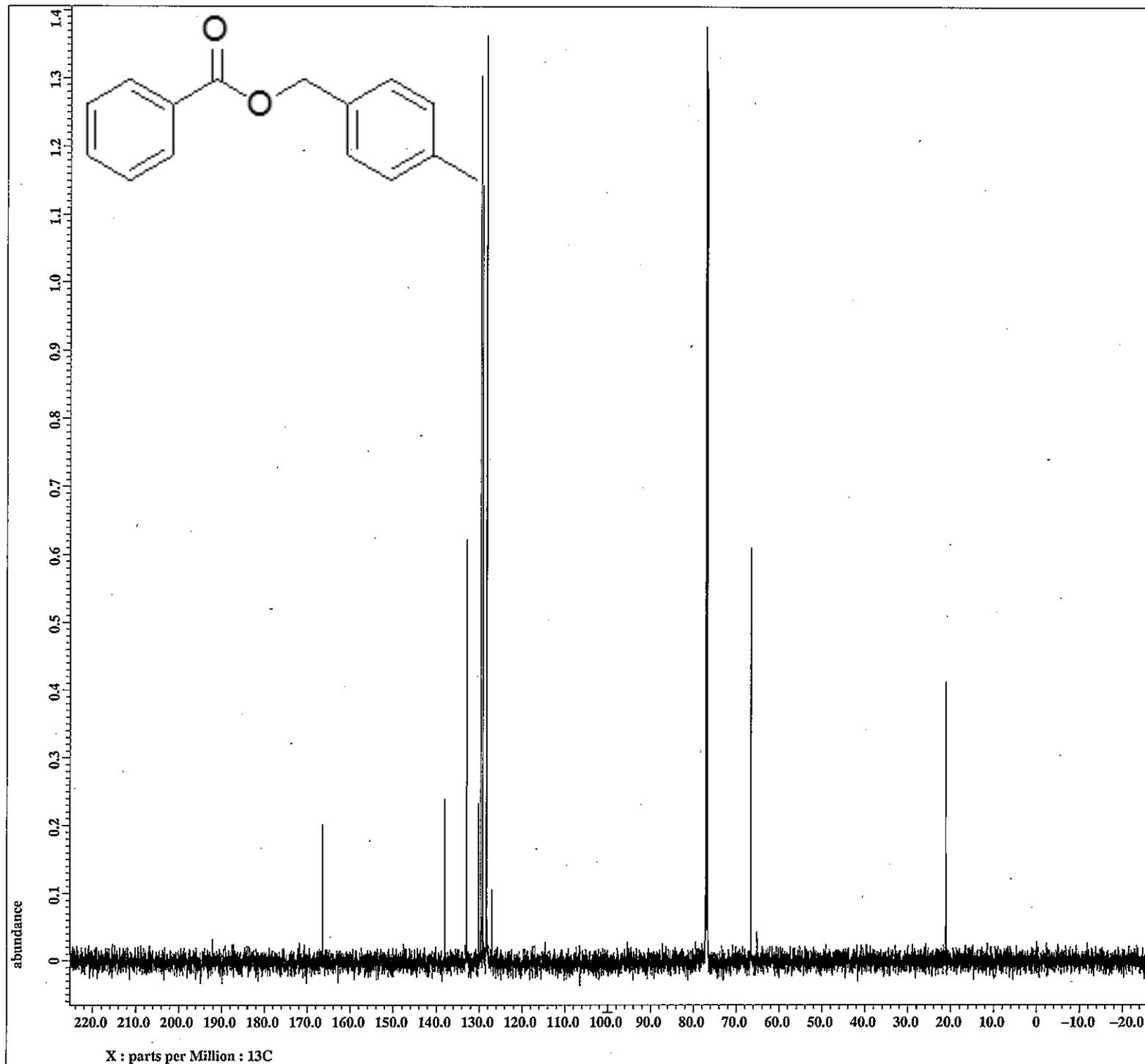


Filename = EXP-T-4-8-Proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = EXP-T-4-8-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:12:20  
Revision\_time = 5-DEC-2012 20:55:02  
Current\_time = 5-DEC-2012 20:55:07

Content = EXP-T-4-8-Proton  
Data\_format = 1D\_COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 44  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19[dC]

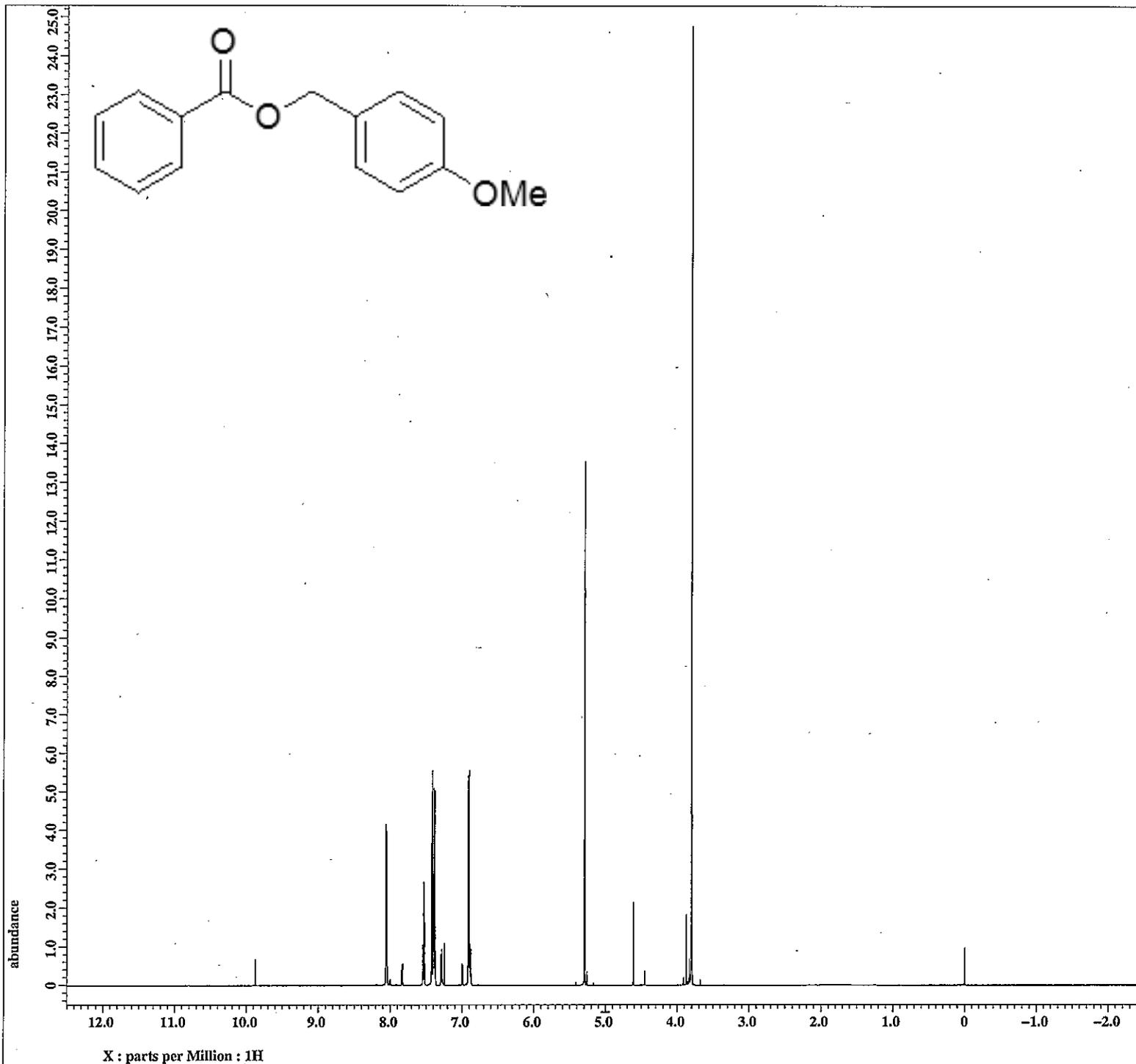


Filename = Exp-T-4-8-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-8-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:17:08  
Revision\_time = 5-DEC-2012 20:55:52  
Current\_time = 5-DEC-2012 20:55:59

Content = Exp-T-4-8-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 91  
Total\_scans = 91

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[dB]  
Irr\_noise = WALTZ  
Decoupling = TRUE  
Initial\_wait = 1[s]  
Noe = TRUE  
Noe\_time = 2[s]  
Recvr\_gain = 60  
Relaxation\_delay = 2[s]  
Repetition\_time = 2.69206016[s]  
Temp\_get = 20[degC]

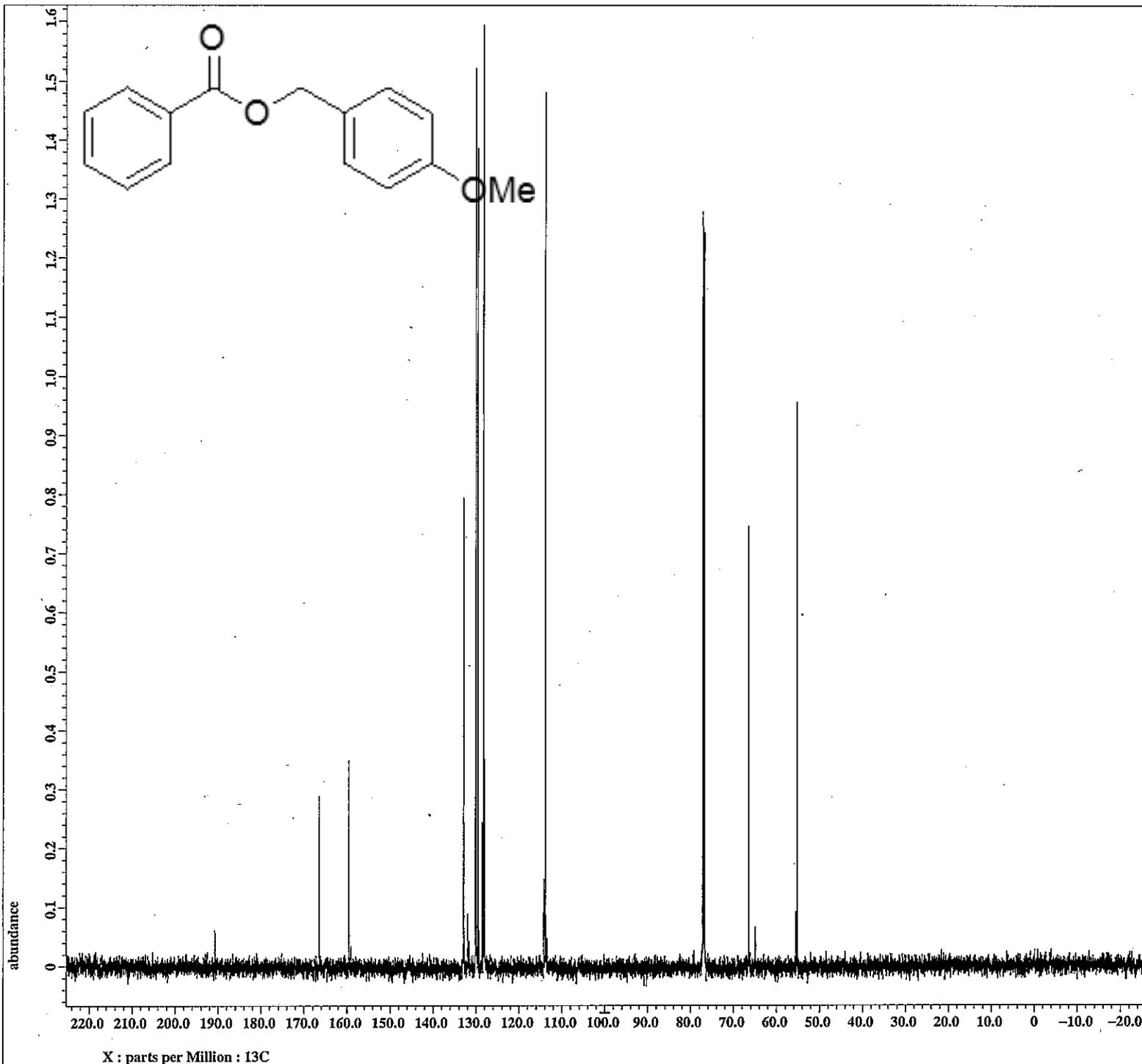


Filename = EXP-T-4-9-Proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = EXP-T-4-9-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:23:10  
Revision\_time = 5-DEC-2012 20:56:32  
Current\_time = 5-DEC-2012 20:56:37

Content = EXP-T-4-9-Proton  
Data\_format = 1D COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[db]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 40  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.5[dc]

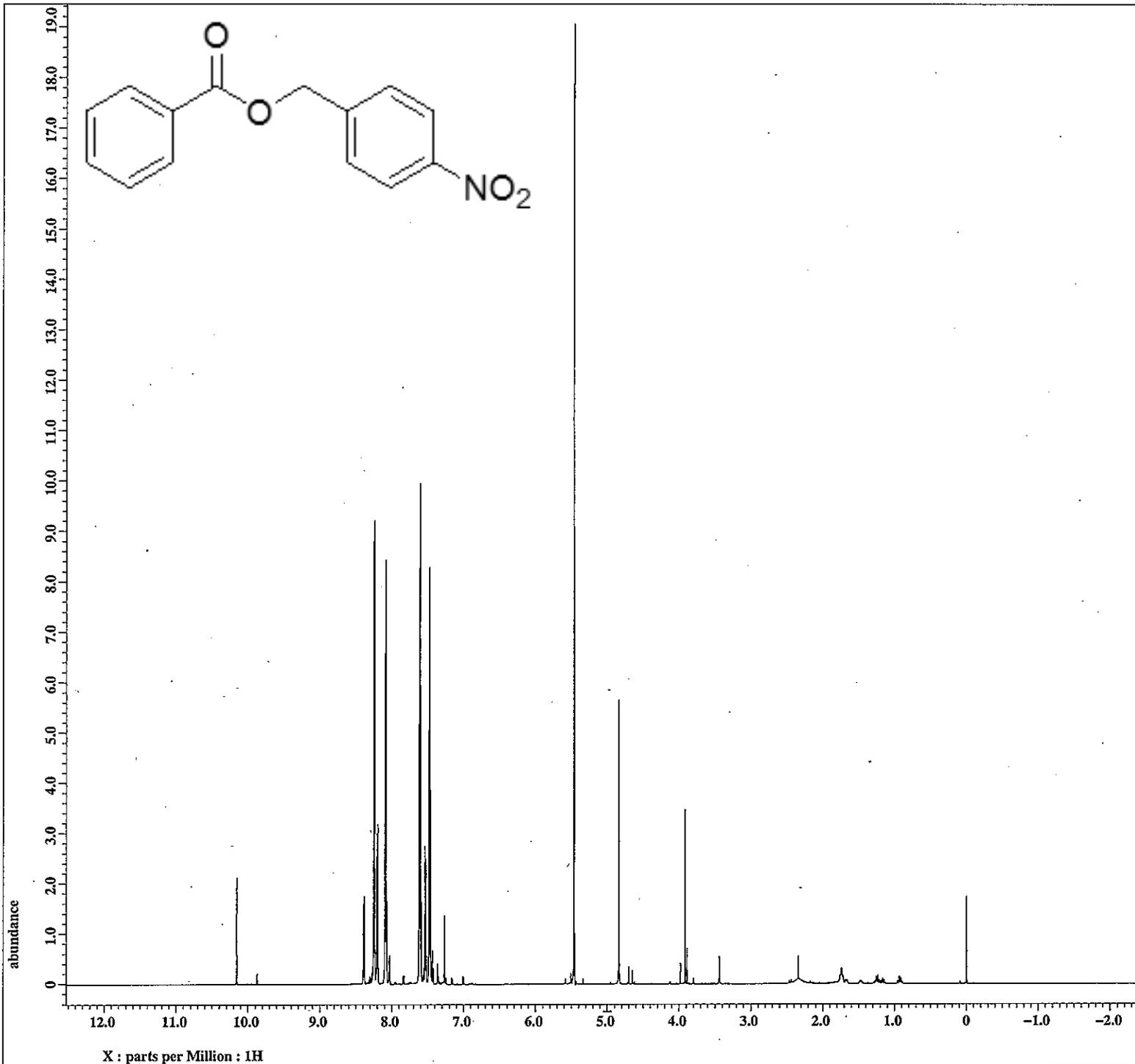
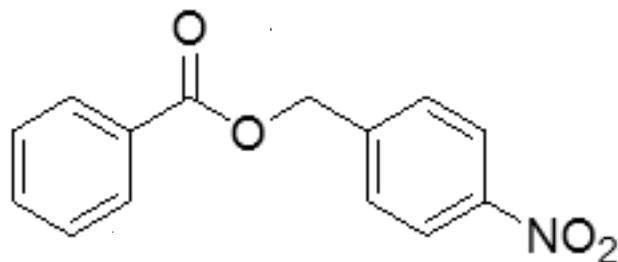


Filename = Exp-T-4-9-carbon-3.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-9-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:28:46  
Revision\_time = 5-DEC-2012 20:57:22  
Current\_time = 5-DEC-2012 20:57:31

Content = Exp-T-4-9-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039 [MHz]  
X\_offset = 100 [ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109 [Hz]  
X\_sweep = 47.34848485 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 109  
Total\_scans = 109

X\_90\_width = 11.3 [us]  
X\_acq\_time = 0.69206016 [s]  
X\_angle = 30 [deg]  
X\_atn = 8 [dB]  
X\_pulse = 3.76666667 [us]  
Irr\_atn\_dec = 19.34784 [dB]  
Irr\_atn\_noe = 19.34784 [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 = 19.7 [dC]

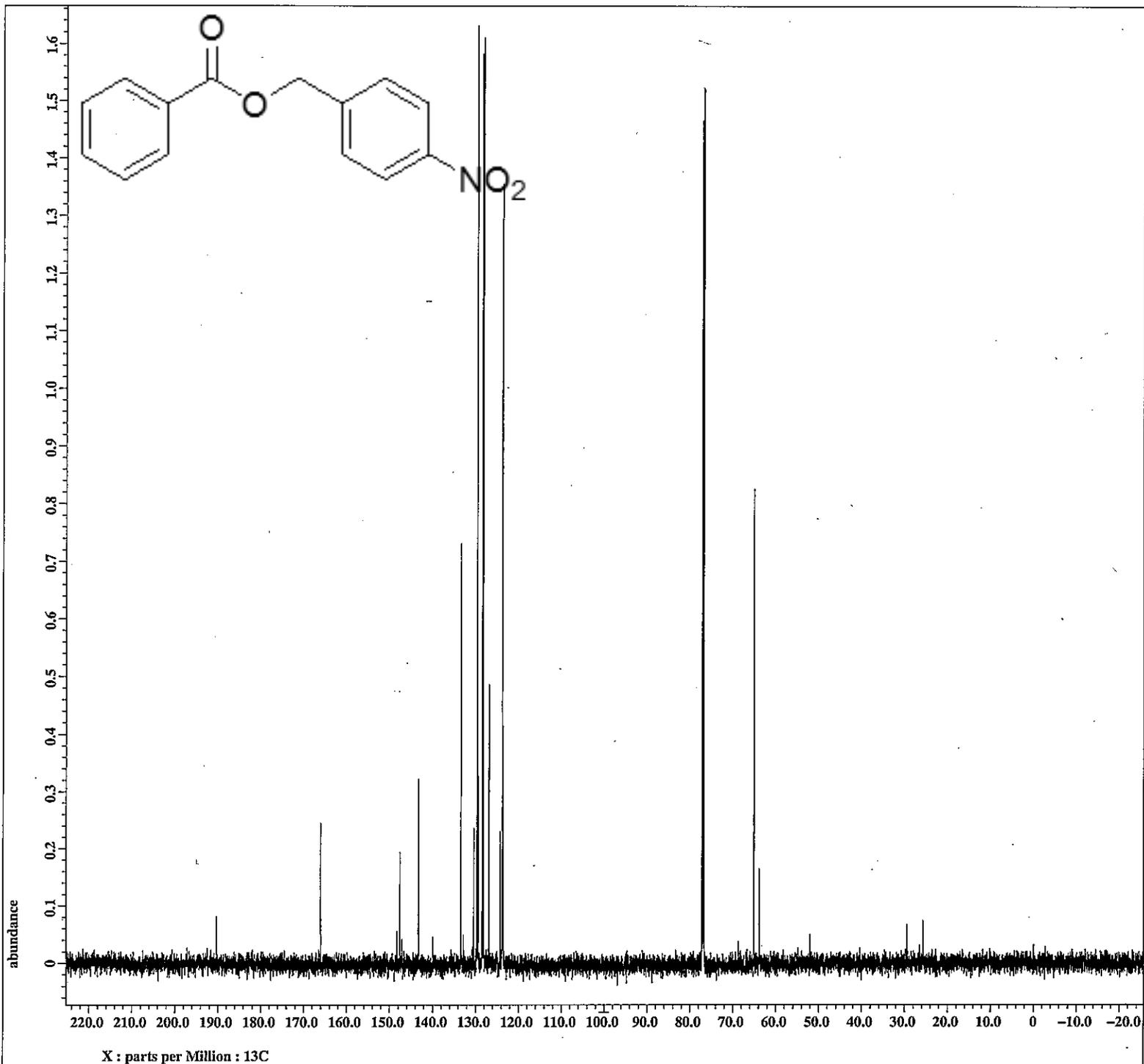


Filename = EXP-T-4-10-Proton-3.j  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = EXP-T-4-10-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:36:17  
Revision\_time = 5-DEC-2012 21:00:13  
Current\_time = 5-DEC-2012 21:00:20

Content = EXP-T-4-10-Proton  
Data\_format = 1D COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_preset = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 44  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.1[degC]

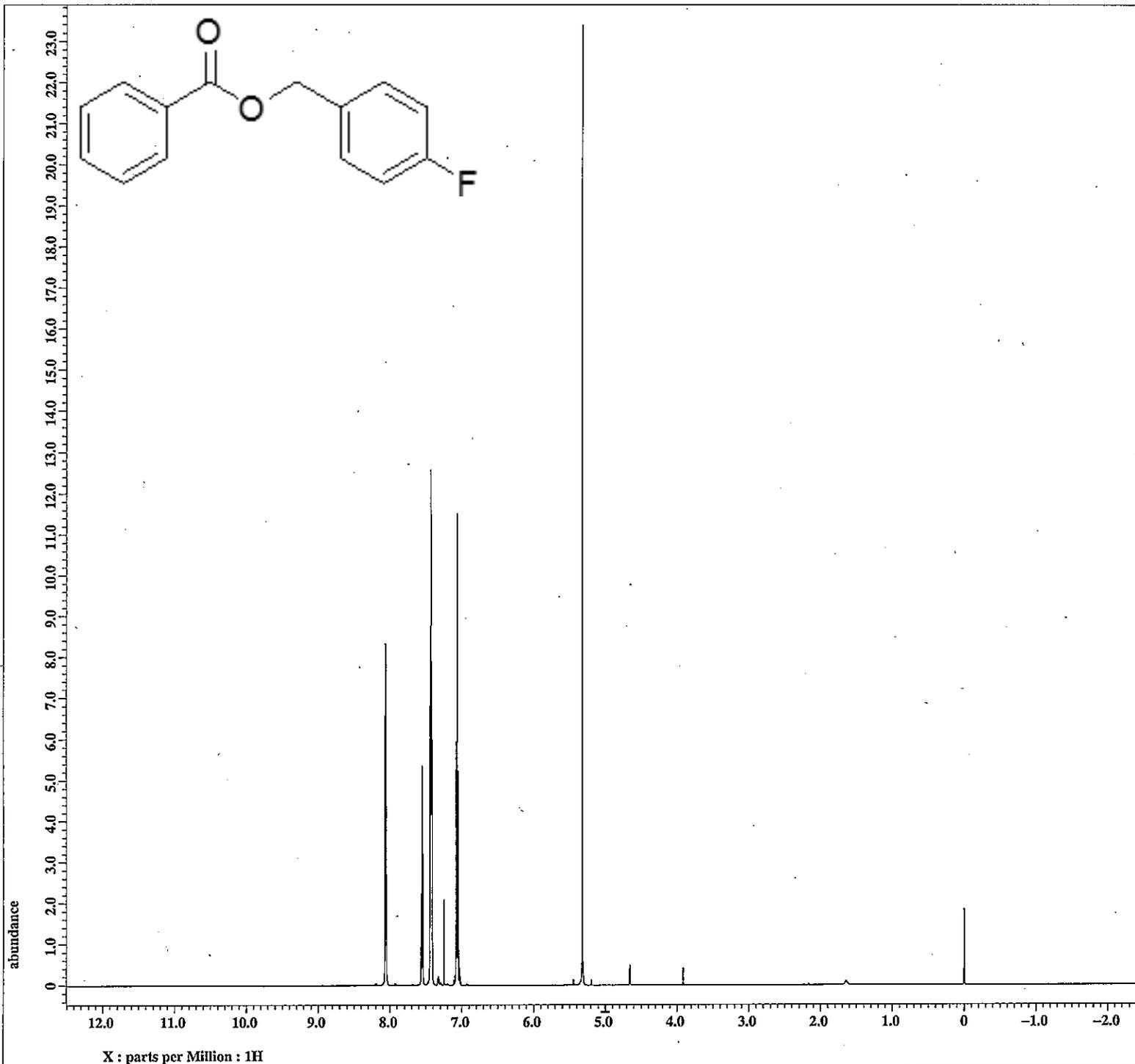


Filename = Exp-T-4-10-carbon-3.j  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-10-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:41:10  
Revision\_time = 5-DEC-2012 21:01:07  
Current\_time = 5-DEC-2012 21:01:15

Content = Exp-T-4-10-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039 [MHz]  
X\_offset = 100 [ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109 [Hz]  
X\_sweep = 47.34848485 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 93  
Total\_scans = 93

X\_90\_width = 11.3 [us]  
X\_acq\_time = 0.69206016 [s]  
X\_angle = 30 [deg]  
X\_atn = 8 [dB]  
X\_pulse = 3.76666667 [us]  
Irr\_atn\_dec = 19.34784 [dB]  
Irr\_atn\_noe = 19.34784 [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 = 19.9 [dC]

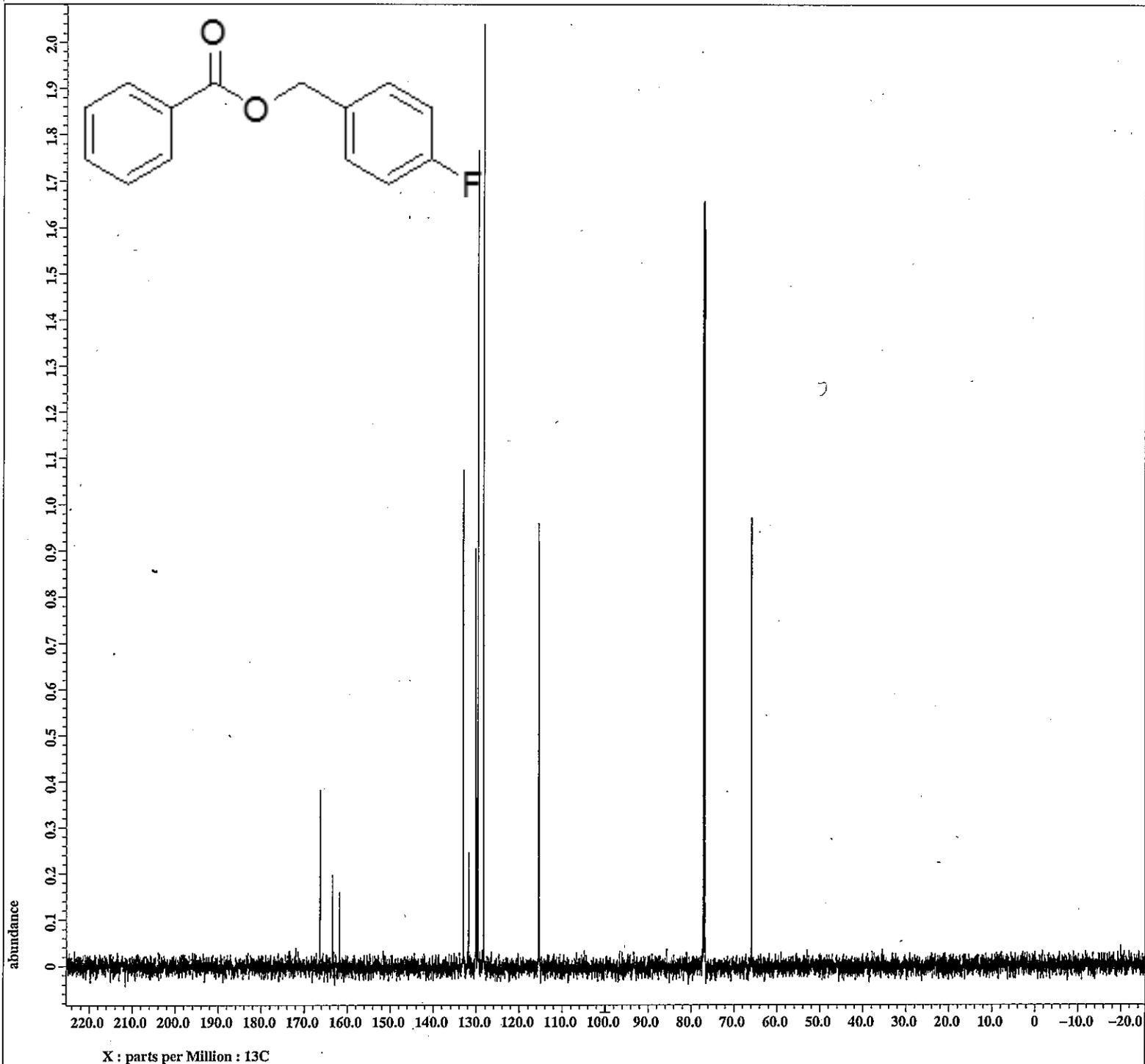


Filename = Exp-T-4-11-Proton-3.j  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-T-4-11-Proton  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:47:51  
Revision\_time = 5-DEC-2012 21:03:40  
Current\_time = 5-DEC-2012 21:03:47

Content = Exp-T-4-11-Proton  
Data\_format = 1D\_COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 44  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 19.3[dc]



Filename = Exp-T-4-11-carbon-3.j  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-T-4-11-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 30-NOV-2012 20:51:05  
Revision\_time = 5-DEC-2012 21:04:31  
Current\_time = 5-DEC-2012 21:04:37

Content = Exp-T-4-11-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 56  
Total\_scans = 56

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[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 = 19.4[degC]

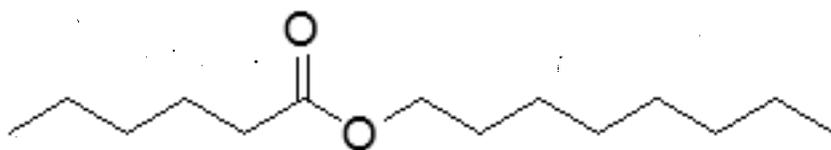
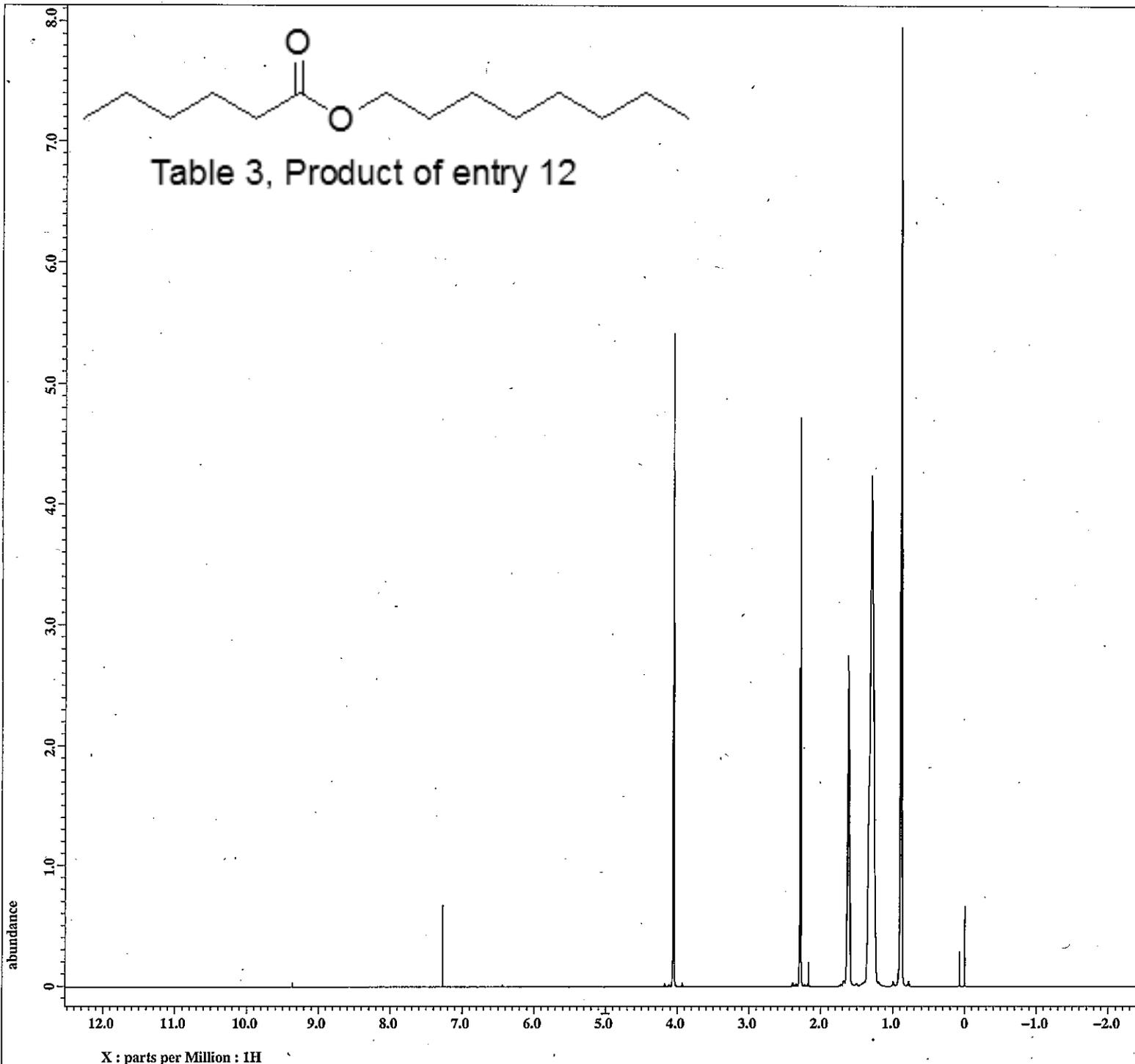


Table 3, Product of entry 12



Filename = Exp-124-1-p-1-proton-  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-124-1-p-1-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 18-FEB-2013 19:26:45  
Revision\_time = 18-FEB-2013 19:54:10  
Current\_time = 18-FEB-2013 19:54:14

Content = Exp-124-1-p-1-proton  
Data\_format = 1D\_COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 34  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 20.5[degC]

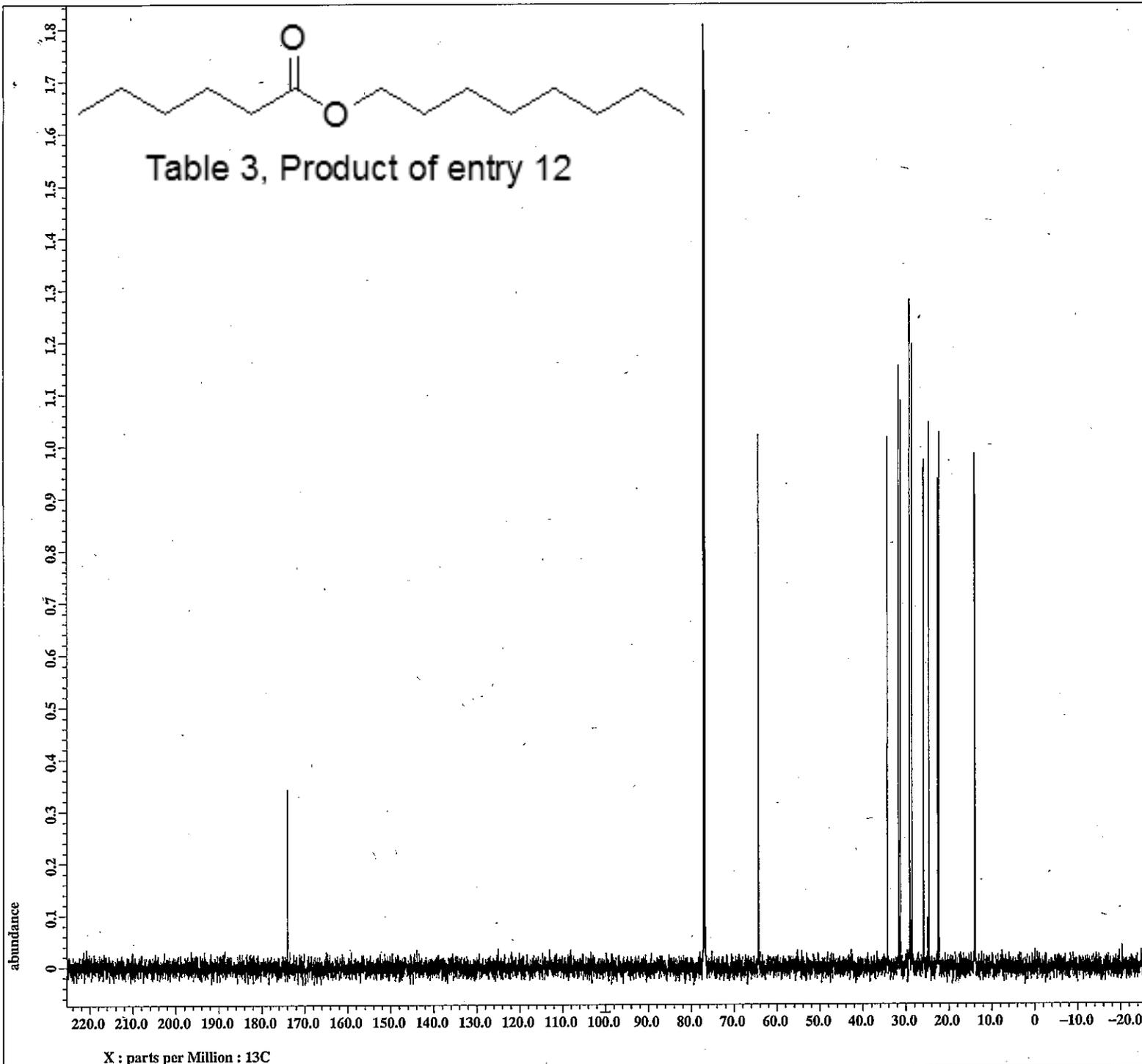


Filename = Exp-124-1-p-1-carbon-  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-124-1-p-1-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 18-FEB-2013 19:30:26  
Revision\_time = 18-FEB-2013 19:54:55  
Current\_time = 18-FEB-2013 19:54:59

Content = Exp-124-1-p-1-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 66  
Total\_scans = 66

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[db]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[db]  
Irr\_atn\_noe = 19.34784[db]  
Irr\_noise = WALTZ  
Decoupling = TRUE  
Initial\_wait = 1[s]  
Noe = TRUE  
Noe\_time = 2[s]  
Recvr\_gain = 60  
Relaxation\_delay = 2[s]  
Repetition\_time = 2.69206016[s]  
Temp\_get = 21.1[dc]



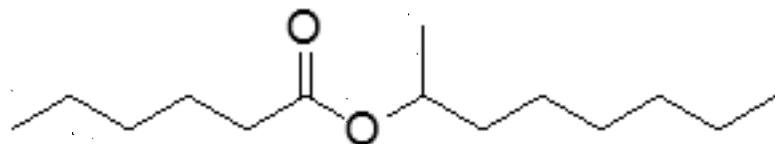
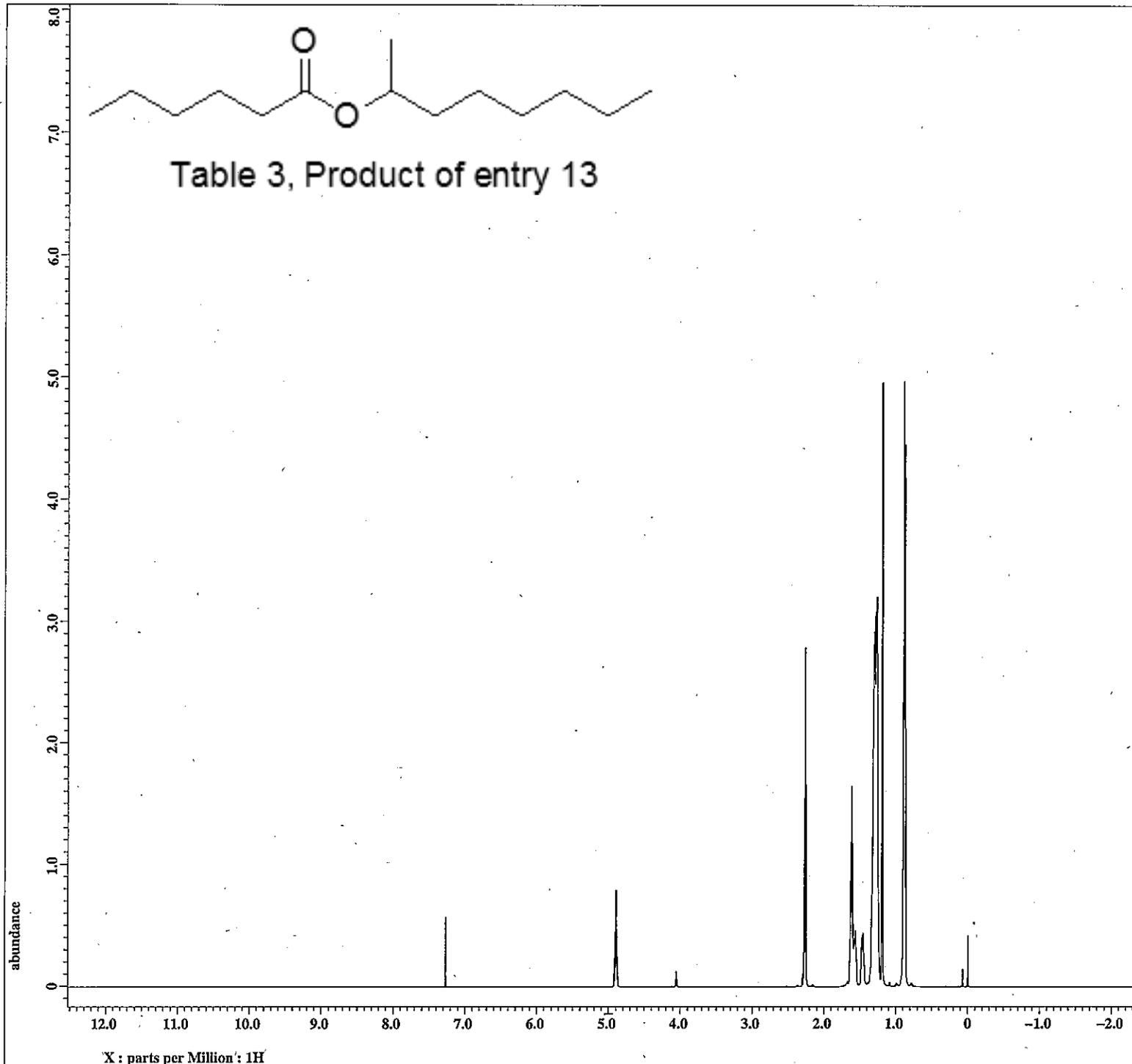


Table 3, Product of entry 13



Filename = Exp-124-3a-proton-3.j  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-124-3a-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 18-FEB-2013 11:52:28  
Revision\_time = 18-FEB-2013 12:22:50  
Current\_time = 18-FEB-2013 12:22:58

Content = Exp-124-3a-proton  
Data\_format = 1D\_COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046[MHz]  
X\_offset = 5[ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284[Hz]  
X\_sweep = 11.26126126[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046[MHz]  
Tri\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4[us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45[deg]  
X\_atn = 3.6[dB]  
X\_pulse = 6.2[us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1[s]  
Recvr\_gain = 34  
Relaxation\_delay = 5[s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 20.6[dc]

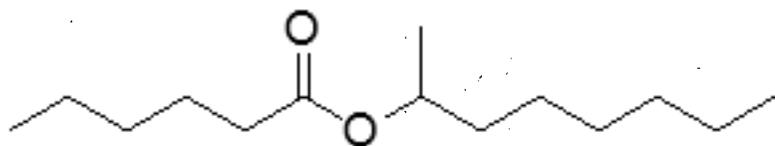
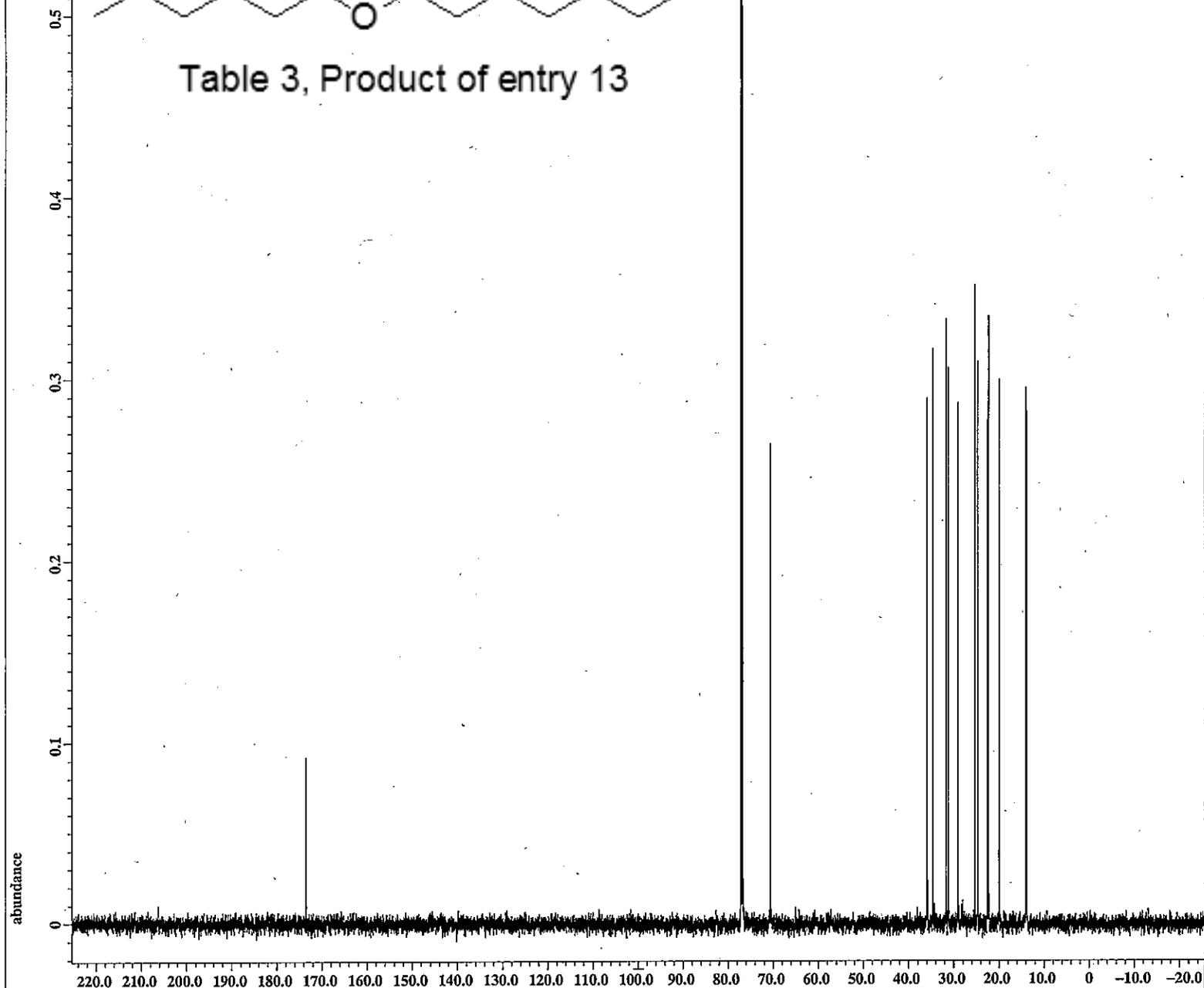


Table 3, Product of entry 13



X : parts per Million : 13C

Filename = Exp-124-3a-carbon-6.j  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-124-3a-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 18-FEB-2013 12:06:06  
Revision\_time = 18-FEB-2013 12:28:21  
Current\_time = 18-FEB-2013 12:28:25

Content = Exp-124-3a-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928 [T] (600[M]  
X\_acq\_duration = 0.69206016 [s]  
X\_domain = 13C  
X\_freq = 150.91343039 [MHz]  
X\_offset = 100 [ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109 [Hz]  
X\_sweep = 47.34848485 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 116.0  
Total\_scans = 116.0

X\_90\_width = 11.3 [us]  
X\_acq\_time = 0.69206016 [s]  
X\_angle = 30 [deg]  
X\_atn = 8 [dB]  
X\_pulse = 3.76666667 [us]  
Irr\_atn\_dec = 19.34784 [dB]  
Irr\_atn\_noe = 19.34784 [dB]  
Irr\_noise = WALTZ  
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 = 20.6 [dC]

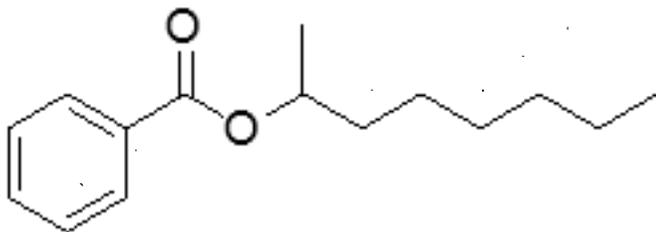
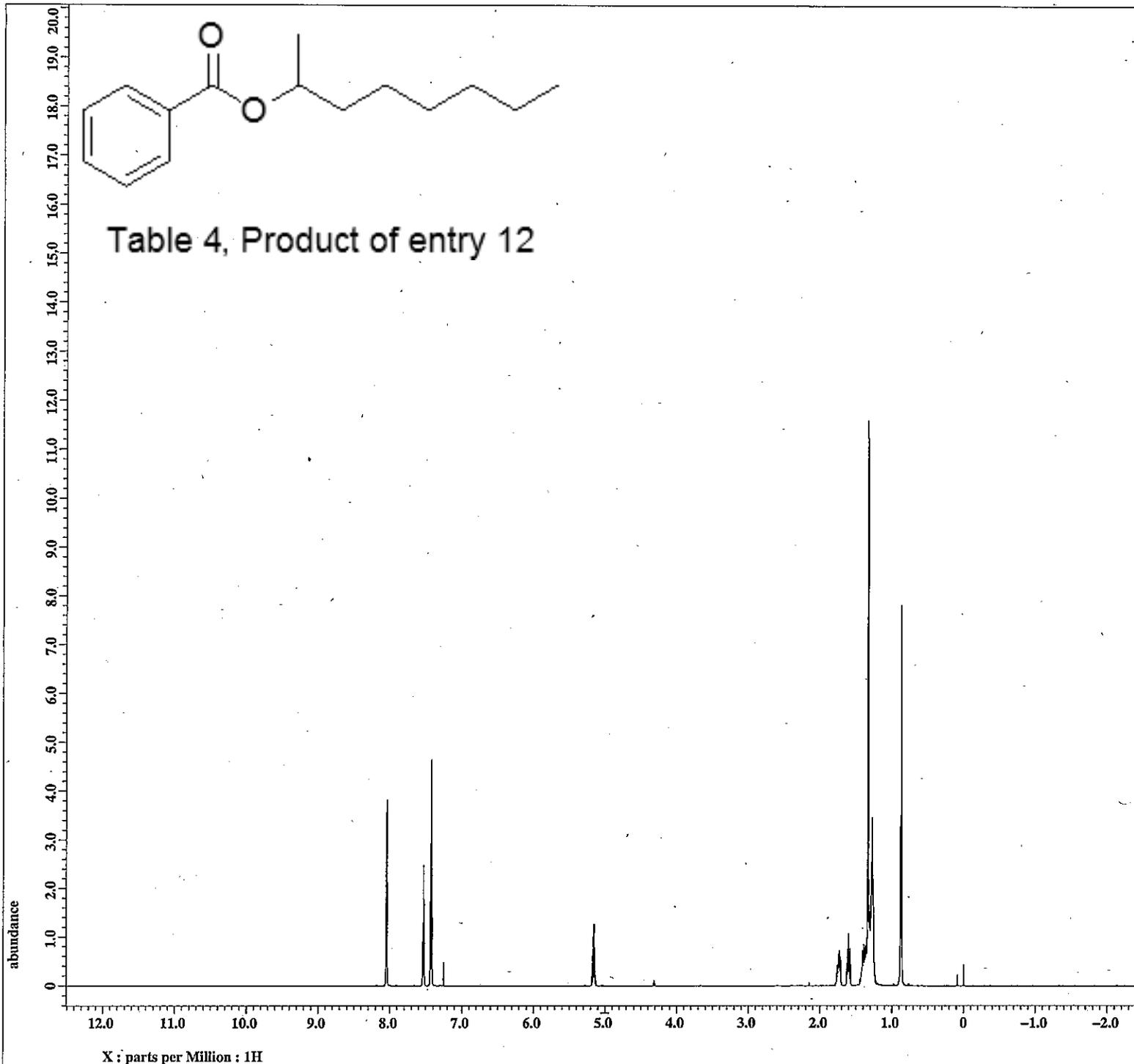


Table 4, Product of entry 12



```
Filename      = Exp-121-3-p-1-proton-
Author       = delta
Experiment    = single_pulse.ex2
Sample_id    = Exp-121-3-p-1-proton
Solvent      = CHLOROFORM-D
Creation_time = 15-FEB-2013 22:23:44
Revision_time = 18-FEB-2013 12:25:56
Current_time  = 18-FEB-2013 12:26:04

Content      = Exp-121-3-p-1-proton
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 600
Spectrometer = DELTA2_NMR

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

X_90_width    = 12.4[us]
X_acq_time    = 1.4548992[s]
X_angle       = 45[deg]
X_atn         = 3.6[dB]
X_pulse       = 6.2[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_preset  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 30
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get      = 20.2[dc]
```

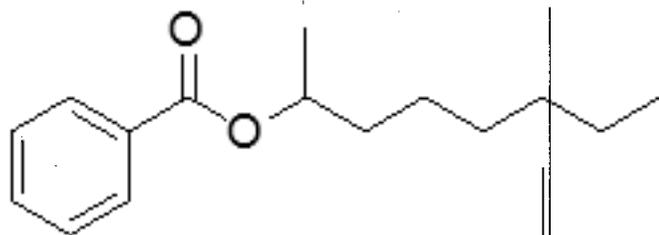
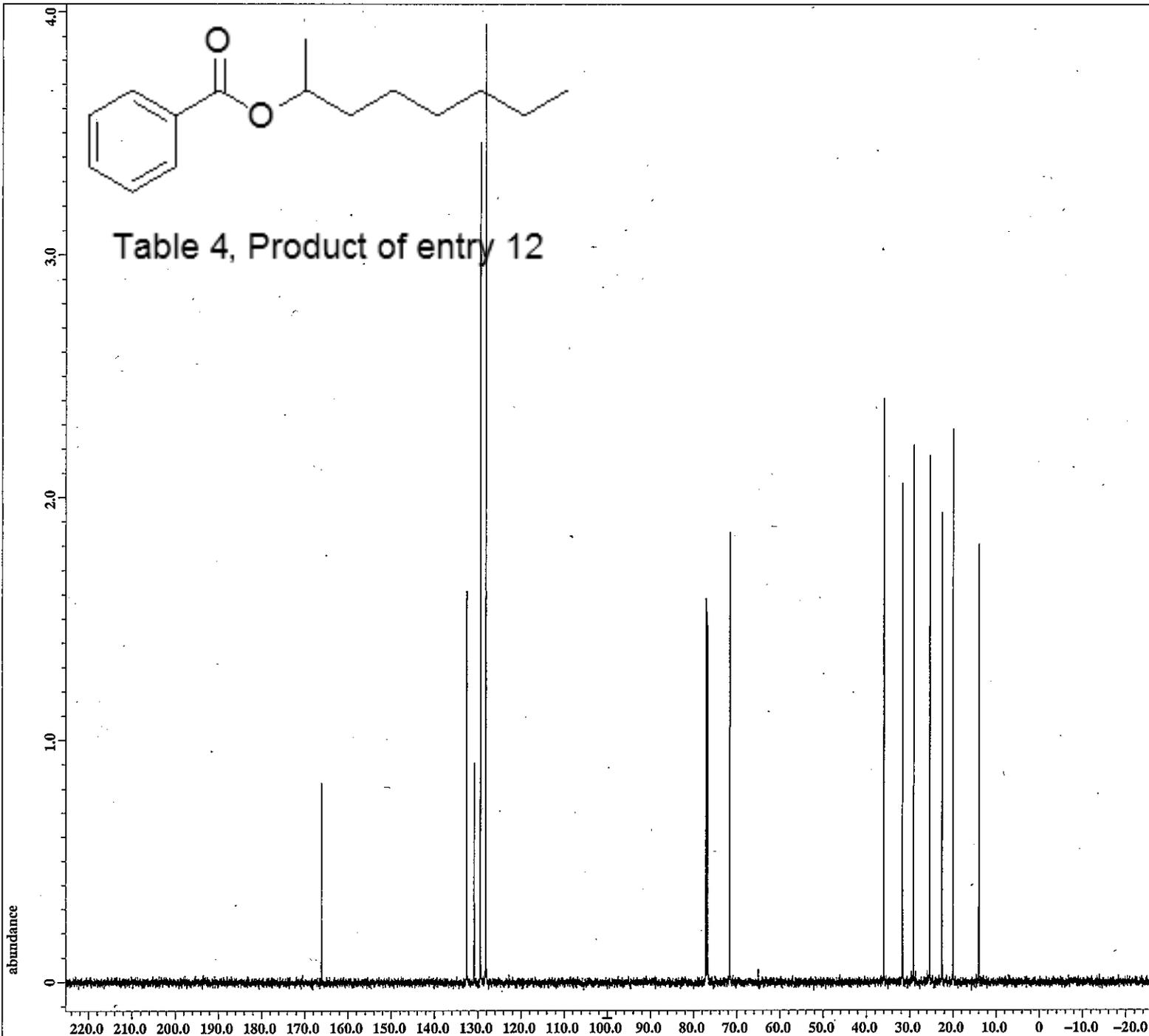


Table 4, Product of entry 12



X : parts per Million : 13C

Filename = Exp-121-3-p-1-carbon-  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-121-3-p-1-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 15-FEB-2013 22:28:32  
Revision\_time = 18-FEB-2013 12:26:42  
Current\_time = 18-FEB-2013 12:26:49

Content = Exp-121-3-p-1-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928 [T] (600[M  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039 [MHz]  
X\_offset = 100 [ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109 [Hz]  
X\_sweep = 47.34848485 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 91  
Total\_scans = 91

X\_90\_width = 11.3 [us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30 [deg]  
X\_atn = 8 [dB]  
X\_pulse = 3.76666667 [us]  
Irr\_atn\_dec = 19.34784 [dB]  
Irr\_atn\_noe = 19.34784 [dB]  
Irr\_noise = WALTZ  
Decoupling = TRUE  
Initial\_wait = 1 [s]  
Noe = TRUE  
Noe\_time = 2 [s]  
Recvr\_gain = 60  
Relaxation\_delay = 2 [s]  
Repetition\_time = 2.69206016[s]  
Temp\_get = 21 [dc]

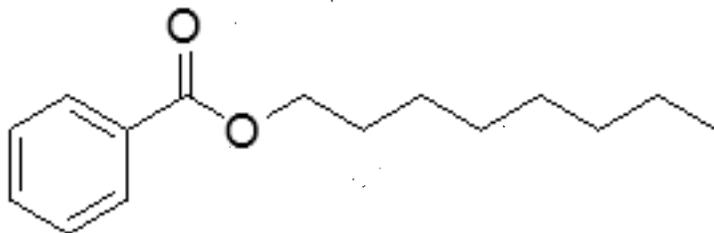
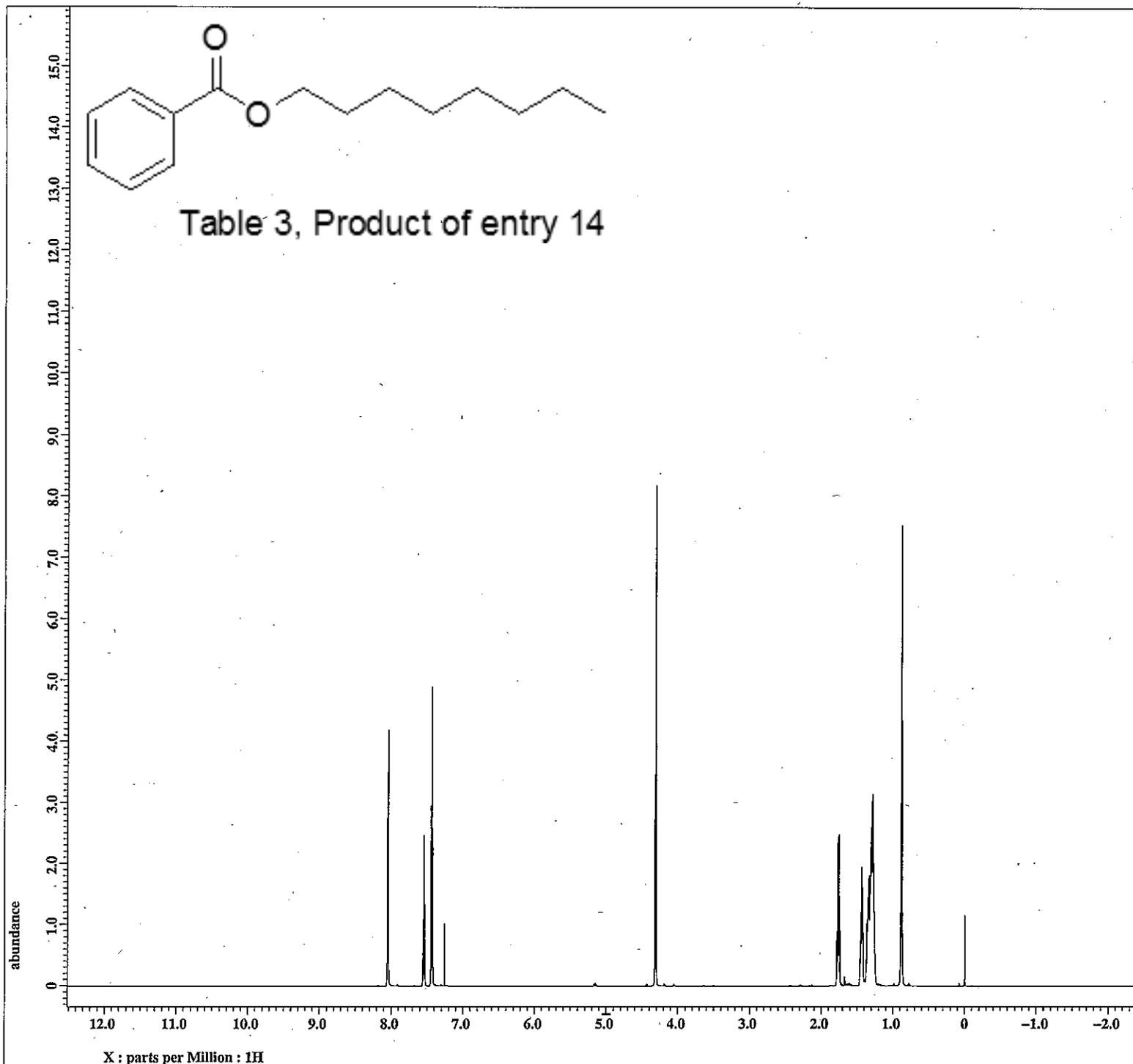


Table 3, Product of entry 14



Filename = Exp-129-2-proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-129-2-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 19-FEB-2013 18:24:22  
Revision\_time = 19-FEB-2013 18:26:52  
Current\_time = 19-FEB-2013 18:27:26

Content = Exp-129-2-proton  
Data\_format = 1D COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 1.4548992[s]  
X\_domain = 1H  
X\_freq = 600.1723046 [MHz]  
X\_offset = 5 [ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284 [Hz]  
X\_sweep = 11.26126126 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046 [MHz]  
Tri\_offset = 5 [ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4 [us]  
X\_acq\_time = 1.4548992[s]  
X\_angle = 45 [deg]  
X\_atn = 3.6 [dB]  
X\_pulse = 6.2 [us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_presat = FALSE  
Initial\_wait = 1 [s]  
Recvr\_gain = 36  
Relaxation\_delay = 5 [s]  
Repetition\_time = 6.4548992[s]  
Temp\_get = 20.1 [dC]

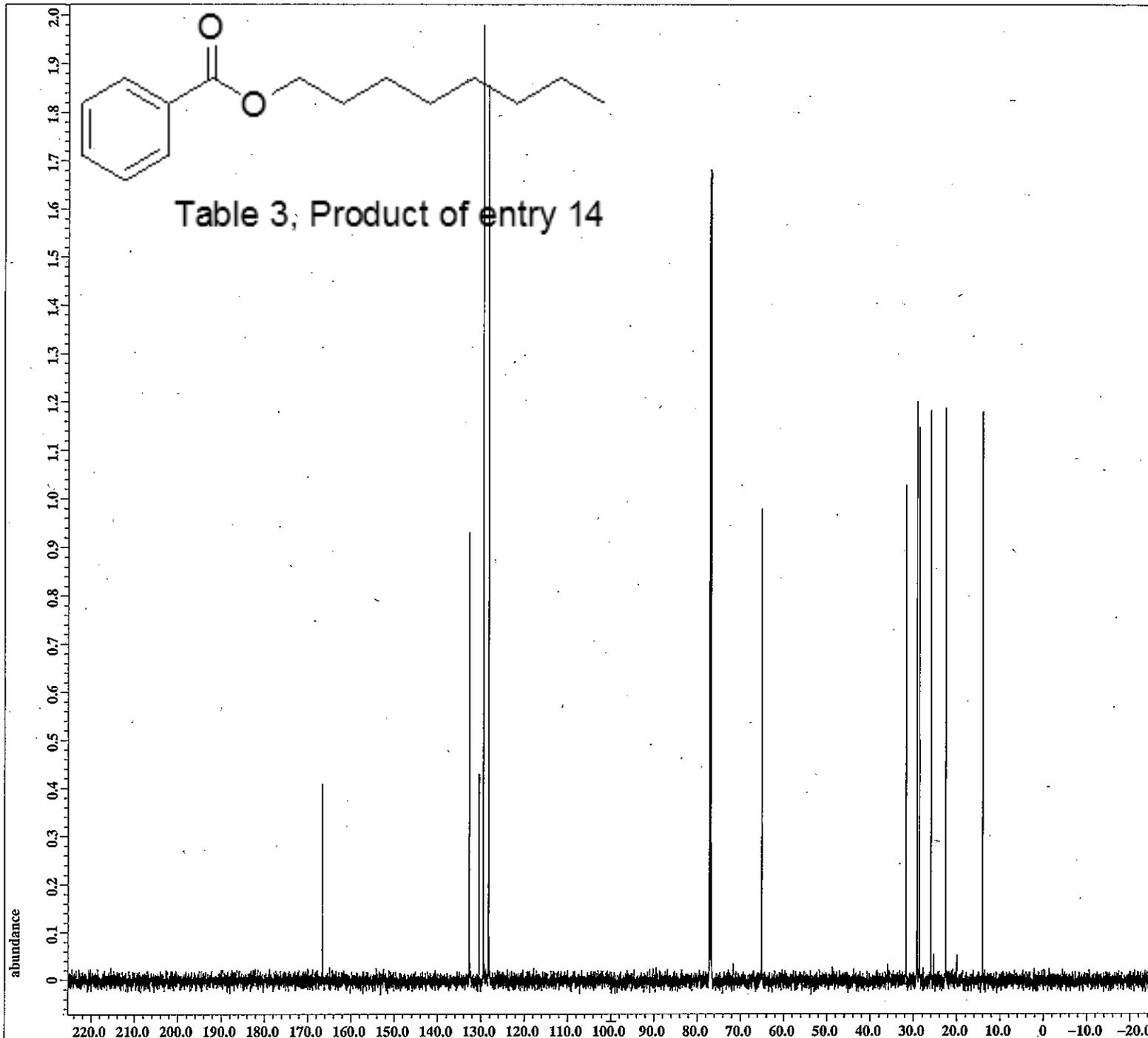


Filename = Exp-129-2-carbon-5.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-129-2-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 19-FEB-2013 18:29:32  
Revision\_time = 19-FEB-2013 18:31:00  
Current\_time = 19-FEB-2013 18:31:03

Content = Exp-129-2-carbon  
Data\_format = 1D\_COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 99  
Total\_scans = 99

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[dB]  
Irr\_noise = WALTZ  
Decoupling = TRUE  
Initial\_wait = 1[s]  
Noe = TRUE  
Noe\_time = 2[s]  
Recvr\_gain = 60  
Relaxation\_delay = 2[s]  
Repetition\_time = 2.69206016[s]  
Temp\_get = 20.7[°C]



X : parts per Million : 13C

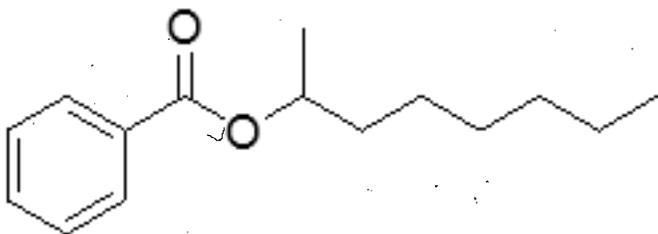
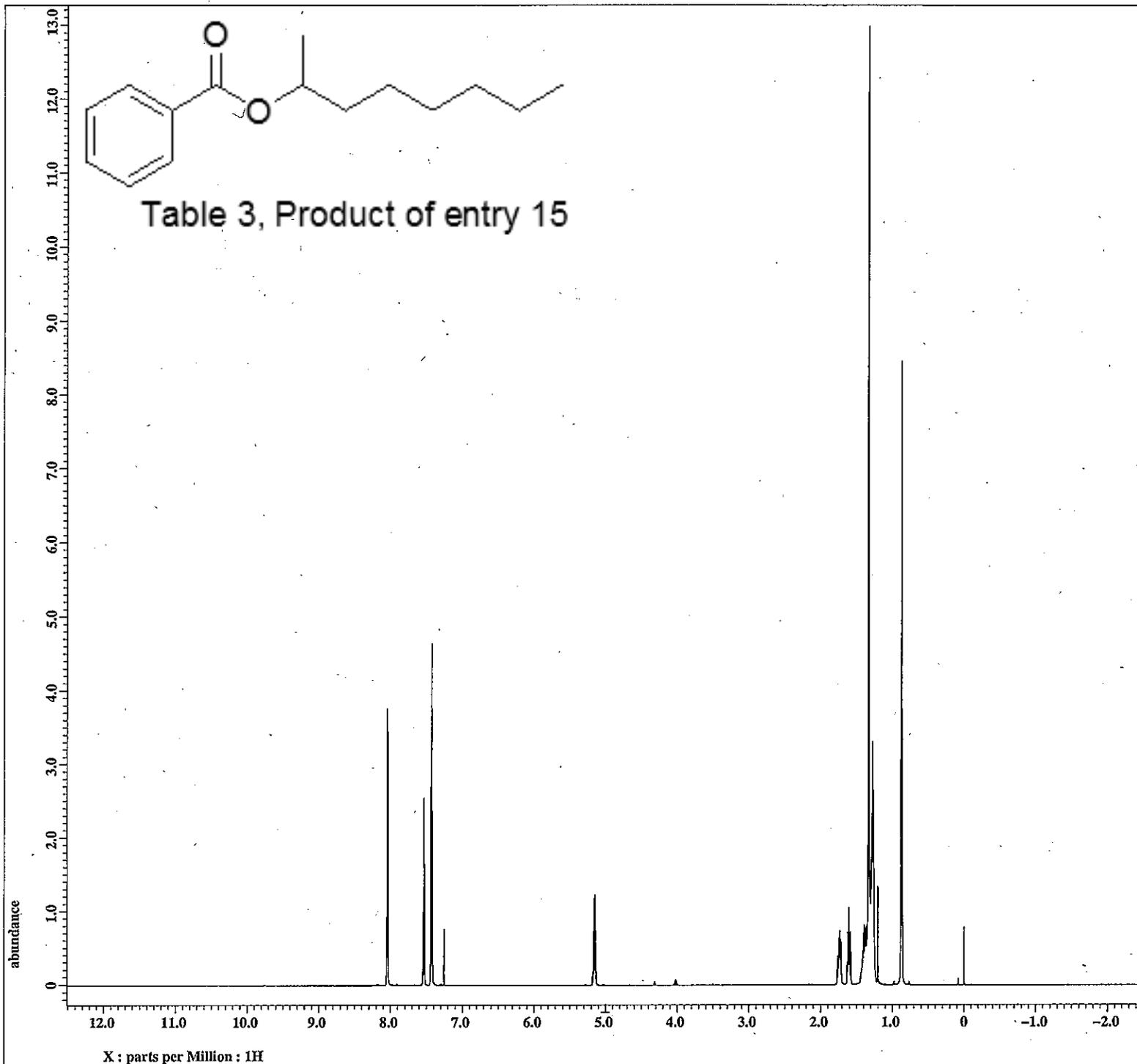


Table 3, Product of entry 15



Filename = Exp-129-4-proton-3.jd  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_id = Exp-129-4-proton  
Solvent = CHLOROFORM-D  
Creation\_time = 19-FEB-2013 18:37:22  
Revision\_time = 19-FEB-2013 18:44:03  
Current\_time = 19-FEB-2013 18:44:07

Content = Exp-129-4-proton  
Data\_format = 1D COMPLEX  
Dim\_size = 13107  
Dim\_title = 1H  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928 [T] (600 [M])  
X\_acq\_duration = 1.4548992 [s]  
X\_domain = 1H  
X\_freq = 600.1723046 [MHz]  
X\_offset = 5 [ppm]  
X\_points = 16384  
X\_prescans = 1  
X\_resolution = 0.68733284 [Hz]  
X\_sweep = 11.26126126 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046 [MHz]  
Irr\_offset = 5 [ppm]  
Tri\_domain = 1H  
Tri\_freq = 600.1723046 [MHz]  
Tri\_offset = 5 [ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 8  
Total\_scans = 8

X\_90\_width = 12.4 [us]  
X\_acq\_time = 1.4548992 [s]  
X\_angle = 45 [deg]  
X\_atn = 3.6 [dB]  
X\_pulse = 6.2 [us]  
Irr\_mode = Off  
Tri\_mode = Off  
Dante\_preset = FALSE  
Initial\_wait = 1 [s]  
Recvr\_gain = 34  
Relaxation\_delay = 5 [s]  
Repetition\_time = 6.4548992 [s]  
Temp\_get = 20.3 [dC]

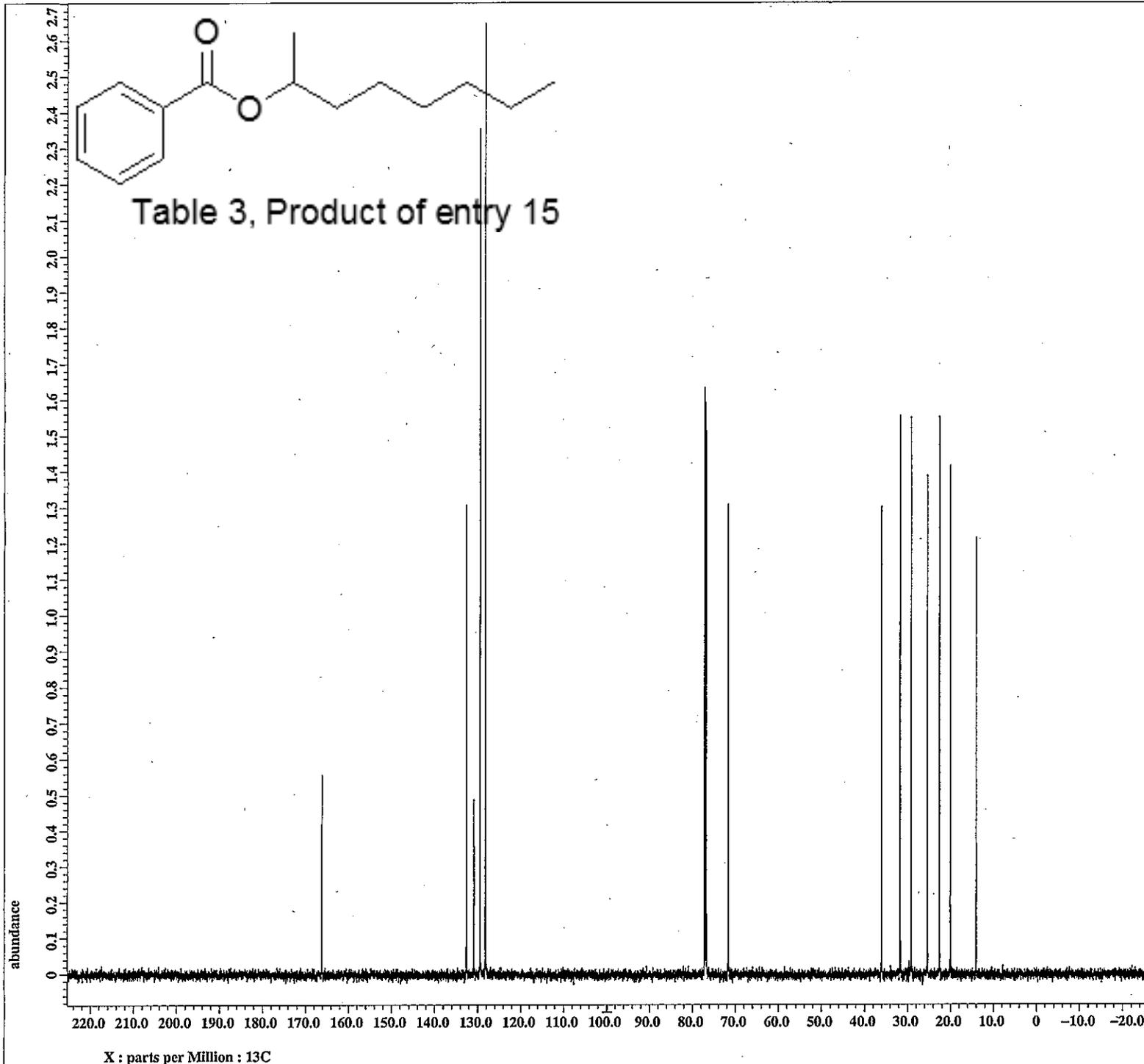


Filename = Exp-129-4-carbon-4.jd  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_id = Exp-129-4-carbon  
Solvent = CHLOROFORM-D  
Creation\_time = 19-FEB-2013 18:44:16  
Revision\_time = 19-FEB-2013 18:45:30  
Current\_time = 19-FEB-2013 18:45:33

Content = Exp-129-4-carbon  
Data\_format = 1D COMPLEX  
Dim\_size = 26214  
Dim\_title = 13C  
Dim\_units = [ppm]  
Dimensions = X  
Site = ECA 600  
Spectrometer = DELTA2\_NMR

Field\_strength = 14.09636928[T] (600[M]  
X\_acq\_duration = 0.69206016[s]  
X\_domain = 13C  
X\_freq = 150.91343039[MHz]  
X\_offset = 100[ppm]  
X\_points = 32768  
X\_prescans = 4  
X\_resolution = 1.44496109[Hz]  
X\_sweep = 47.34848485[kHz]  
Irr\_domain = 1H  
Irr\_freq = 600.1723046[MHz]  
Irr\_offset = 5[ppm]  
Clipped = FALSE  
Mod\_return = 1  
Scans = 138  
Total\_scans = 138

X\_90\_width = 11.3[us]  
X\_acq\_time = 0.69206016[s]  
X\_angle = 30[deg]  
X\_atn = 8[dB]  
X\_pulse = 3.76666667[us]  
Irr\_atn\_dec = 19.34784[dB]  
Irr\_atn\_noe = 19.34784[dB]  
Irr\_noise = WALTZ  
Decoupling = TRUE  
Initial\_wait = 1[s]  
Noe = TRUE  
Noe\_time = 2[s]  
Recvr\_gain = 60  
Relaxation\_delay = 2[s]  
Repetition\_time = 2.69206016[s]  
Temp\_get = 21.1[dc]



X : parts per Million : 13C