Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Efficient and selective oxidation of alcohols to carbonyl compounds at room temperature by ruthenium complex and hydrogen peroxide

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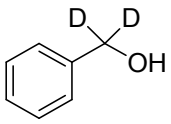
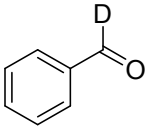
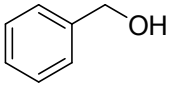
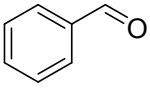
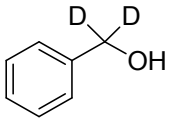
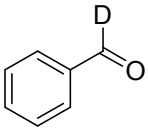
# Supporting Information

Table S1 Effect of temperature variation on the observed rate constants[a]

| Entry | T/K | $k_{obs}$ ($\times 10^3$/min$^{-1}$) |
|---|---|---|
| 1 | 293 | 4.65 |
| 2 | 298 | 6.81 |
| 3 | 303 | 9.30 |
| 4 | 308 | 13.58 |
| 5 | 313 | 18.74 |

[a][Sub] = 2.0 $\times 10^{-2}$ mol/L, [Cat] = 2.0 $\times 10^{-5}$ mol/L, [$H_2O_2$] = 6.0 $\times 10^{-2}$ mol/L

Table S2. Oxidation of deuterated and non-deuterated benzyl alcohol with $H_2O_2$ catalyzed by Ru(mpbp)(pydic)[a]

| Entry | Substrate | Product | Time/min | Conv./% | Yield/% |
|---|---|---|---|---|---|
| 1 |  |  | 60 | 12 | 12 |
| 2[b] |  |  | 60 | 99 | 99 |
| |  |  | | 18 | 18 |

[a]Substrate (1 mmol), catalyst (0.1 mol%), acetonitrile (2 mL), $H_2O_2$ (3.0 equiv.), 25 $^{o}$C.

[b]Benzyl alchol (0.5 mmol), deuterated benzyl alcohol (0.5 mmol).

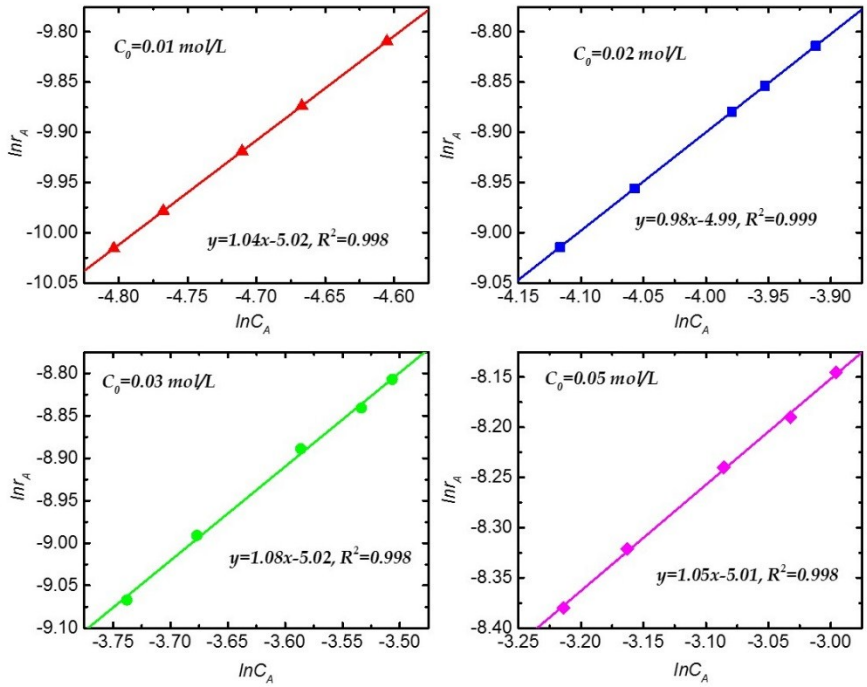



Figure S1 The logarithmic plot beween reaction rate and concentration of benzyl alcohol.

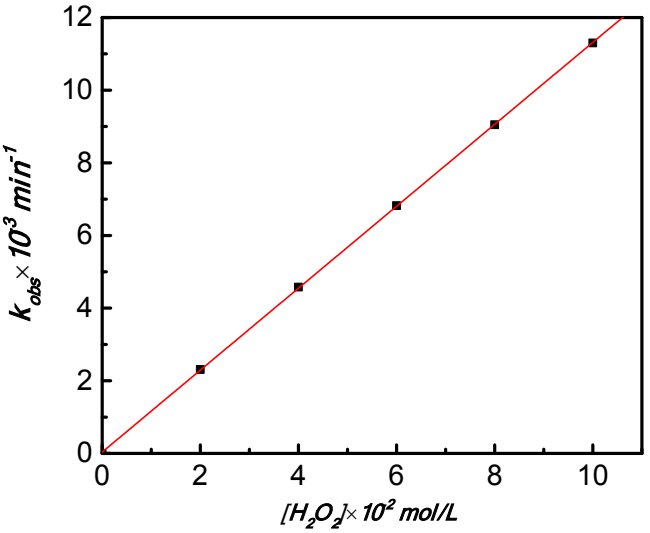



Figure S2. The linear plot of $k_{obs}$ vs $[H_2O_2]$ confirms the first order reaction with respect to $[H_2O_2]$, 298K, [Sub] = 2.0 $\times 10^{-2}$ mol/L, [Cat] = 2.0 $\times 10^{-5}$ mol/L.

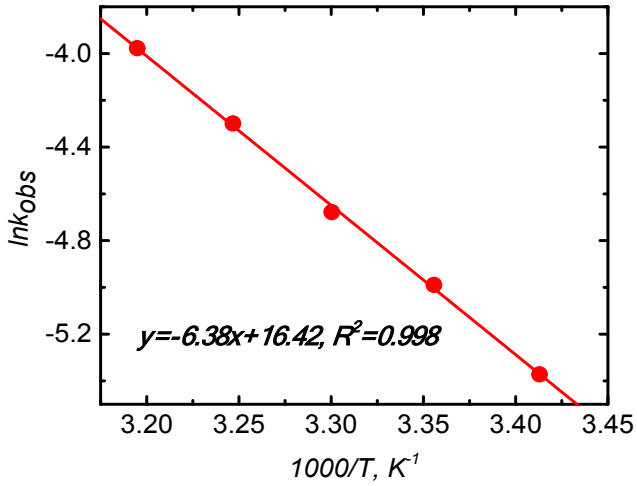



Figure S3. Arrhnius plots of the rate constants for the oxidation of benzyl alcohol.

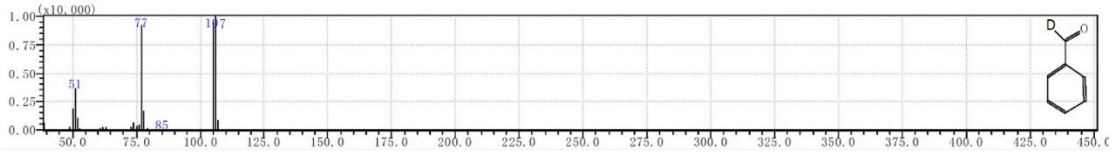
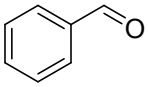
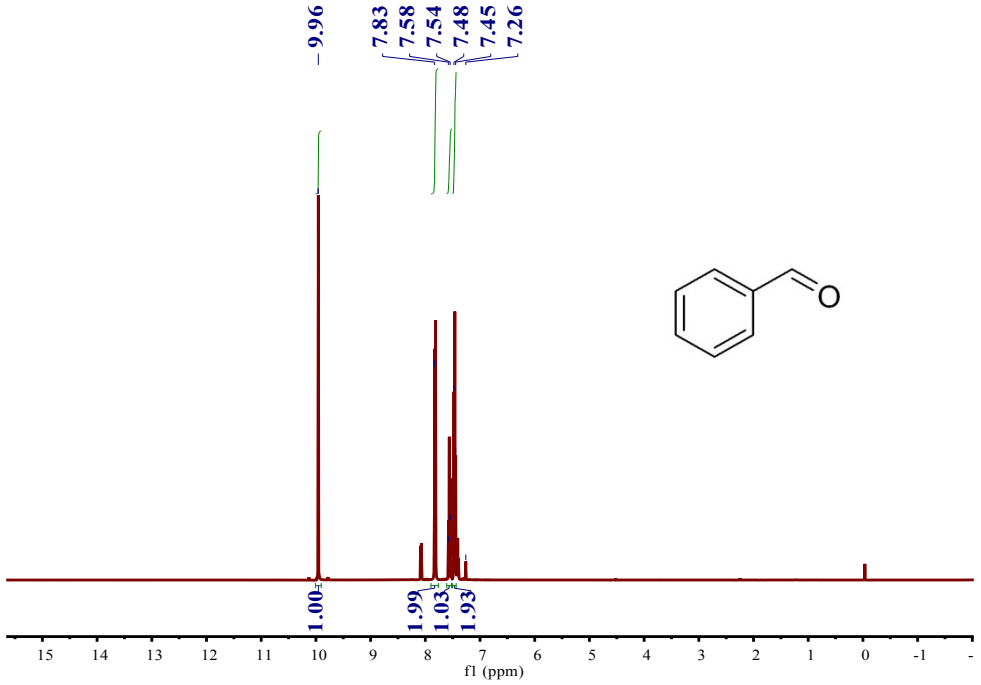



Figure S4. The mass spectrum of deuterated benzaldehyde

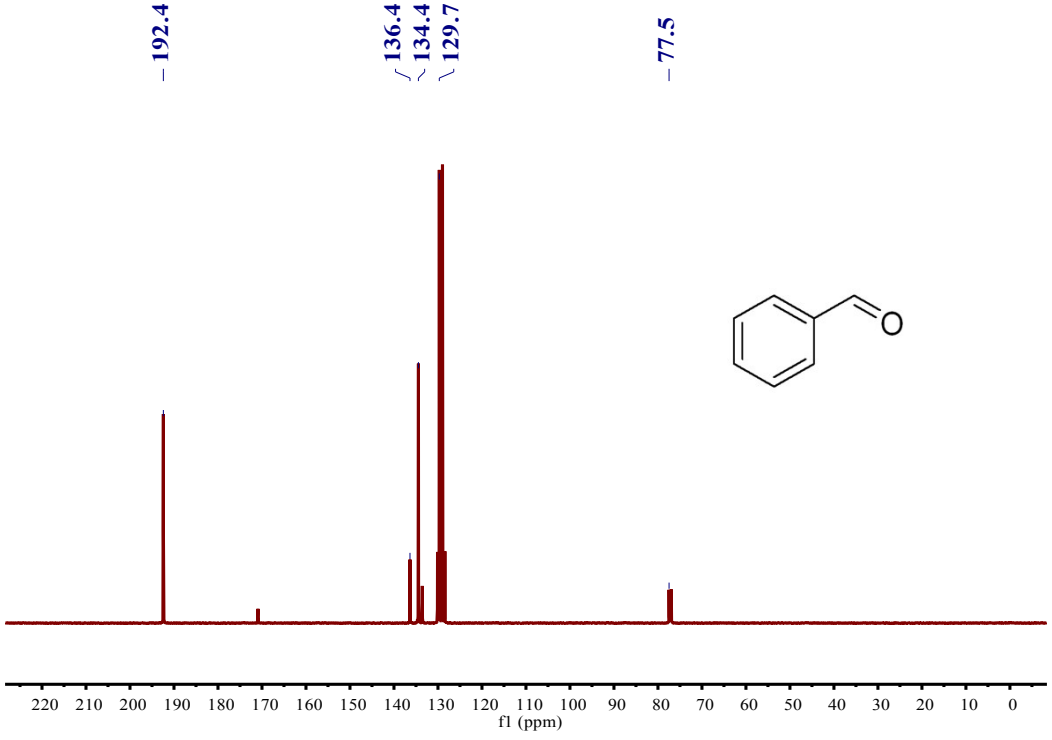
# Spetral data:

**Compound 1:** 

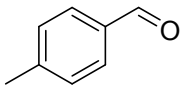
$^{1}$H NMR (500 MHz, $CDCl_3$): δ 9.96 (s, 1H), 7.83 (d, J = 8.0 Hz, 2H), 7.58-7.54 (m, 1H), 7.48-7.45 (m, 2H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 192.4, 136.4, 134.4, 129.7.



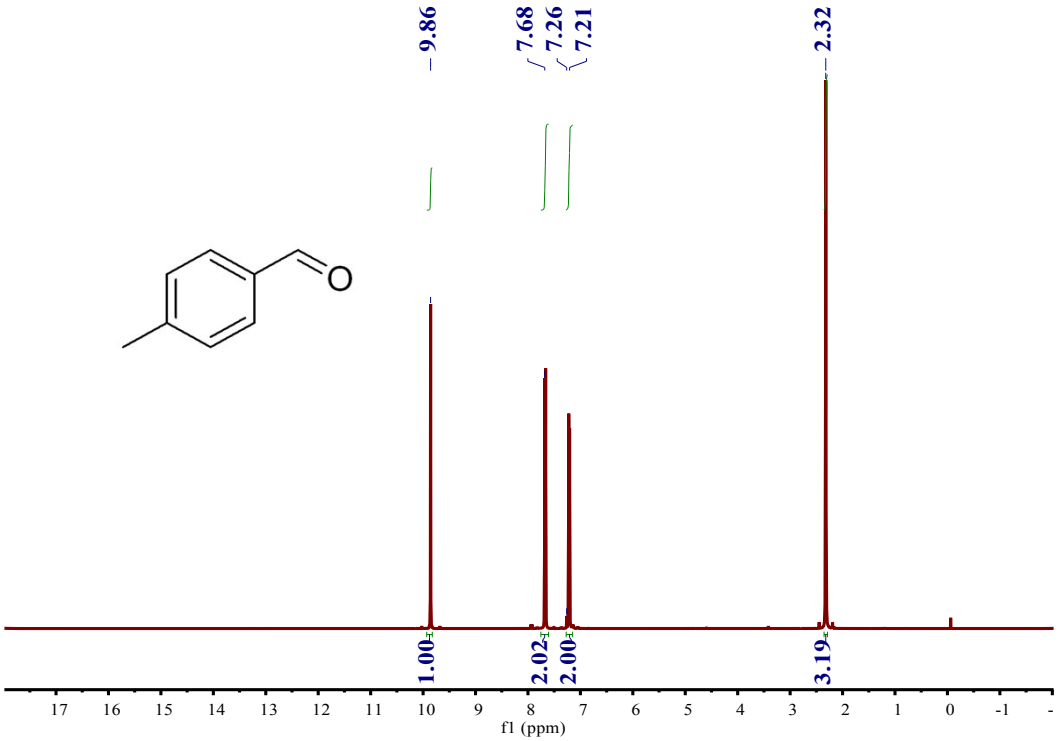

$^{1}$H NMR Spectrum of Compound 1



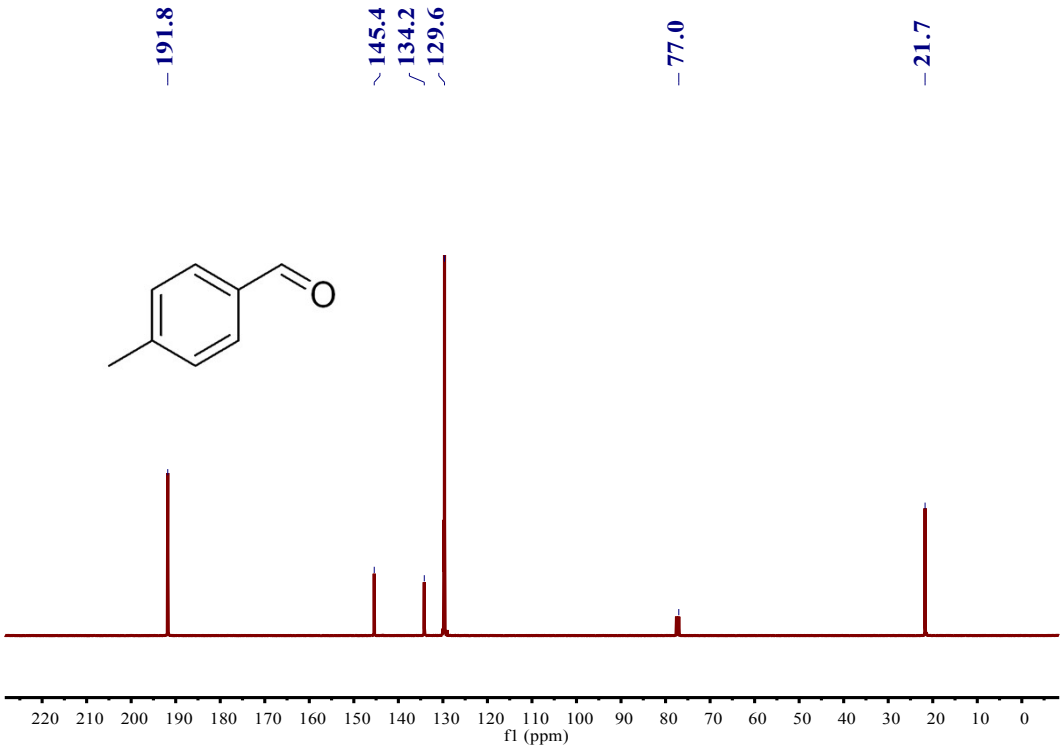

$^{13}$C NMR Spectrum of Compound 1

**Compound 2:** 

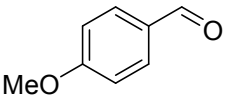
$^{1}$H NMR (500 MHz, $CDCl_3$): δ 9.86 (s, 1H), 7.68 (d, J = 8.1 Hz, 2H), 7.21 (d, J = 7.8 Hz, 2H), 2.32 (s, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 191.8, 145.4, 134.2, 129.6, 21.7.



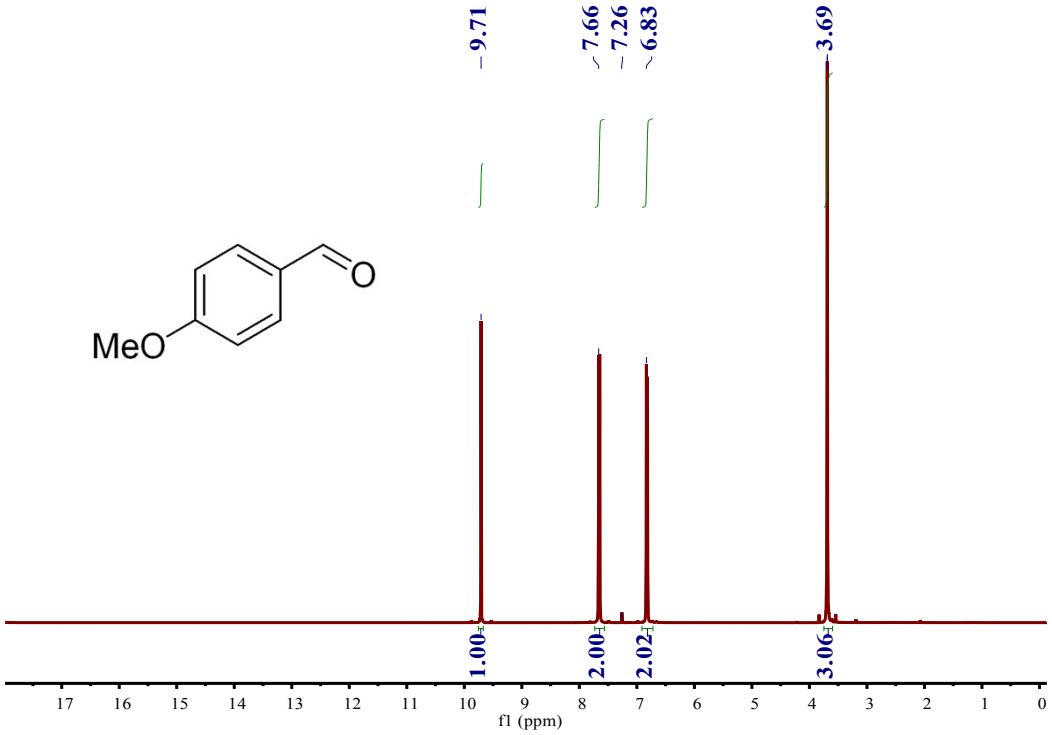

$^{1}$H NMR Spectrum of Compound 2



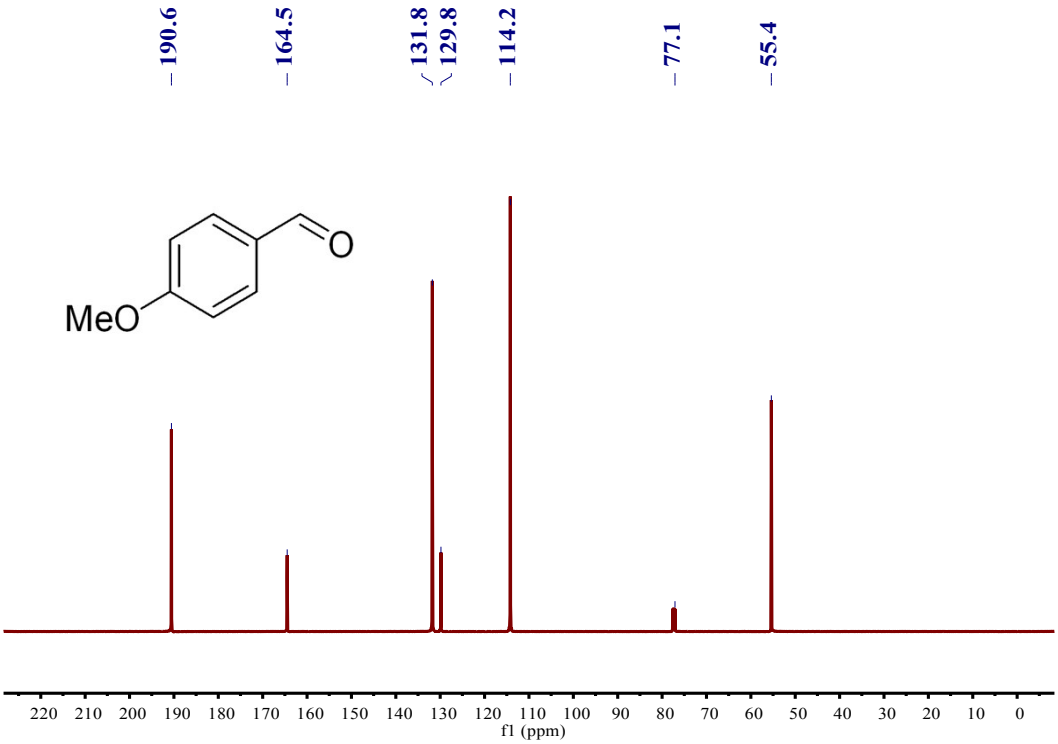

$^{13}$C NMR Spectrum of Compound 2

**Compound 3:** 

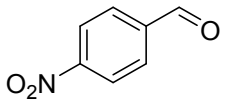

$^{1}$H NMR (500 MHz, $CDCl_3$): δ 9.71 (s, 1H), 7.66 (d, J = 8.0 Hz, 2H), 6.83 (d, J = 7.8 Hz, 2H), 3.69 (s, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 190.6, 164.5, 131.8, 129.8, 114.2, 55.4.




$^{1}$H NMR Spectrum of Compound 3

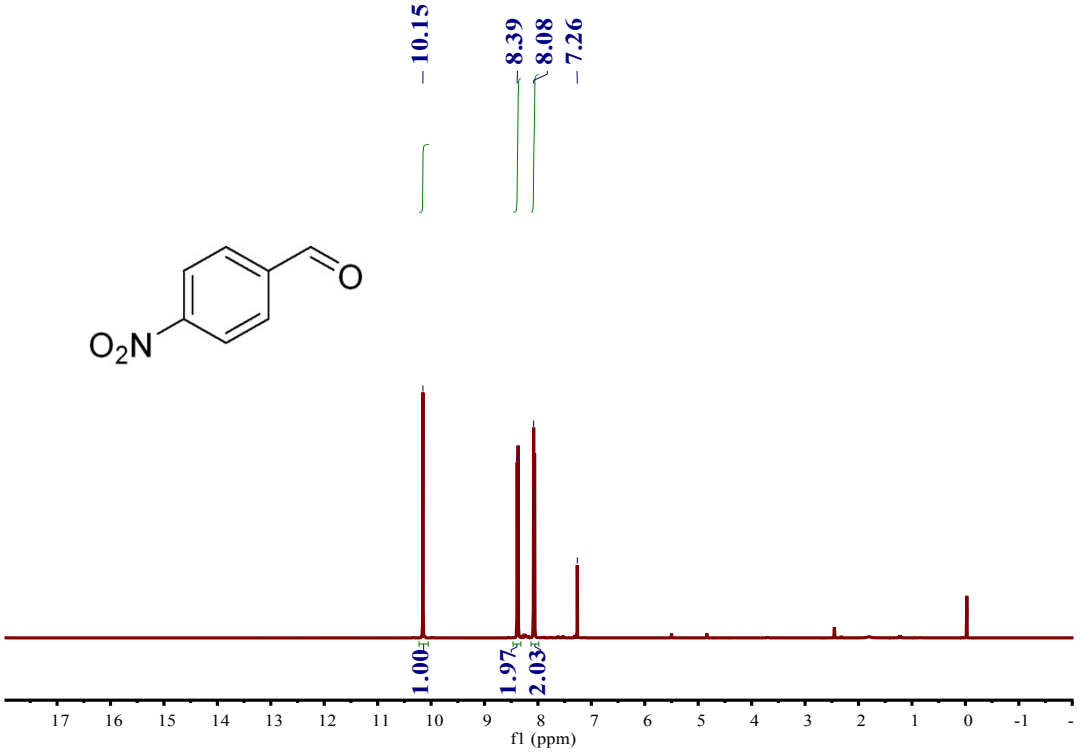



$^{13}$C NMR Spectrum of Compound 3

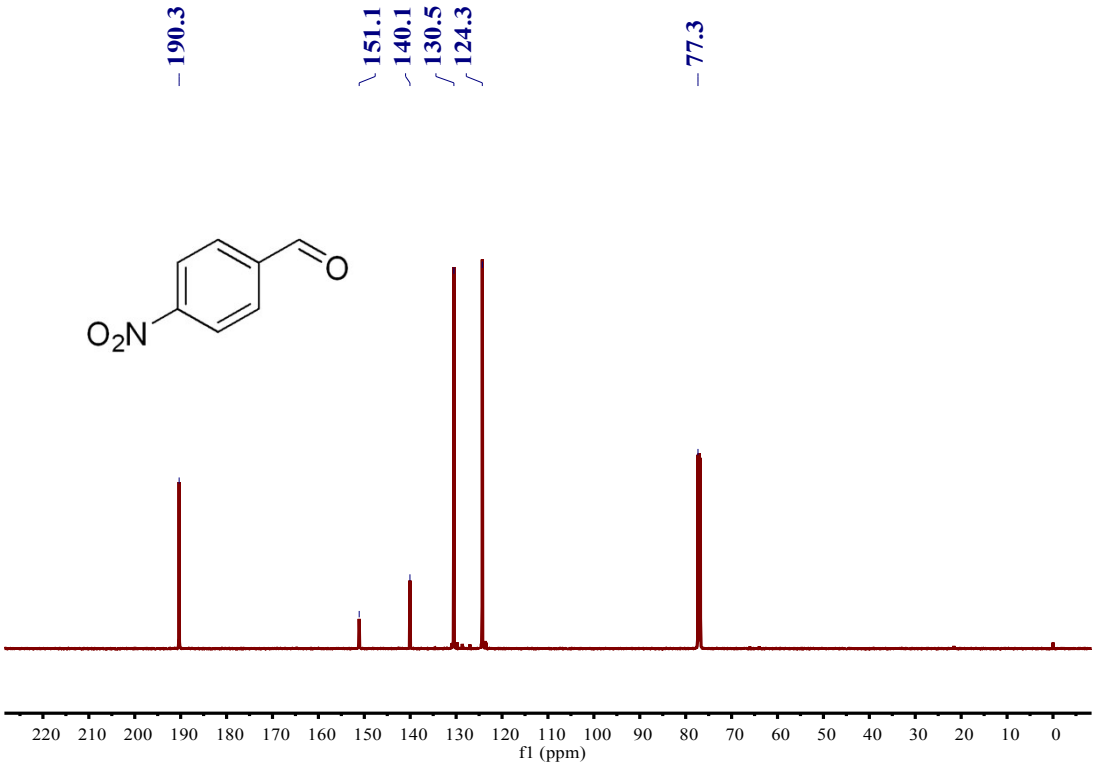
**Compound 4:** 

$^{1}$H NMR (500 MHz, $CDCl_3$): δ 10.15 (s, 1H), 8.39 (d, J = 8.0 Hz, 2H), 8.08 (d, J = 8.0 Hz, 2H).

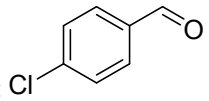
$^{13}$C NMR (125 MHz, $CDCl_3$): δ 190.3, 151.1, 140.1, 130.5, 124.3.



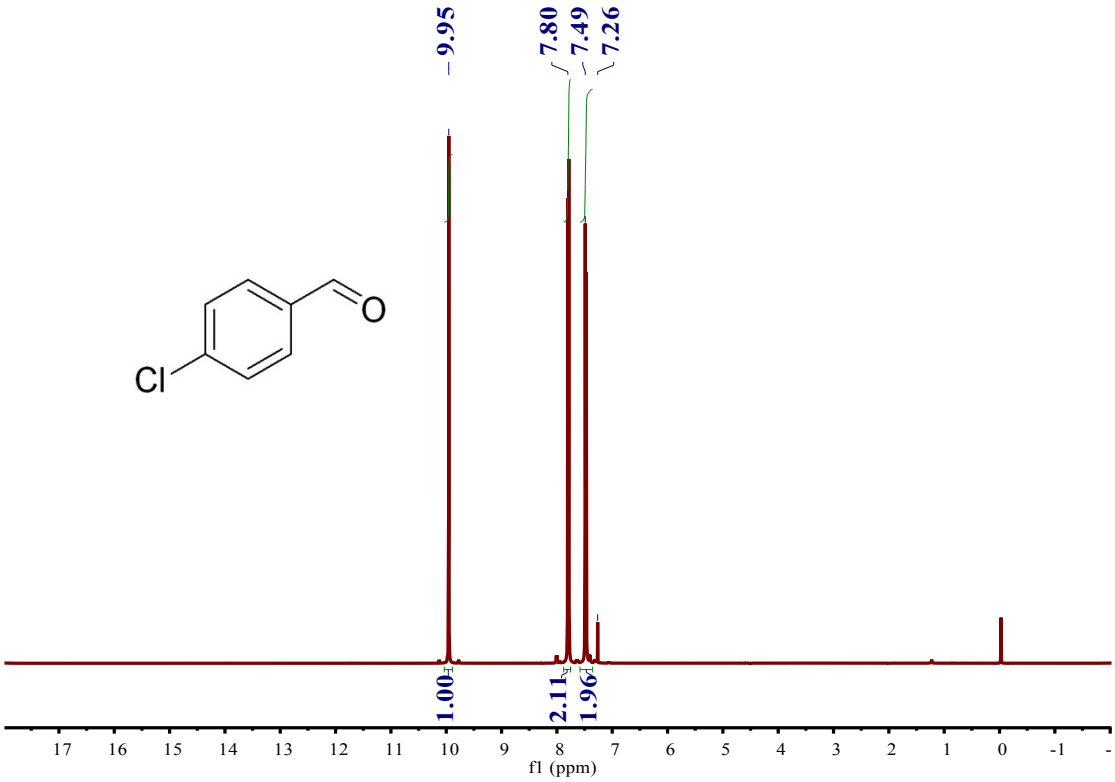

$^{1}$H NMR Spectrum of Compound 4



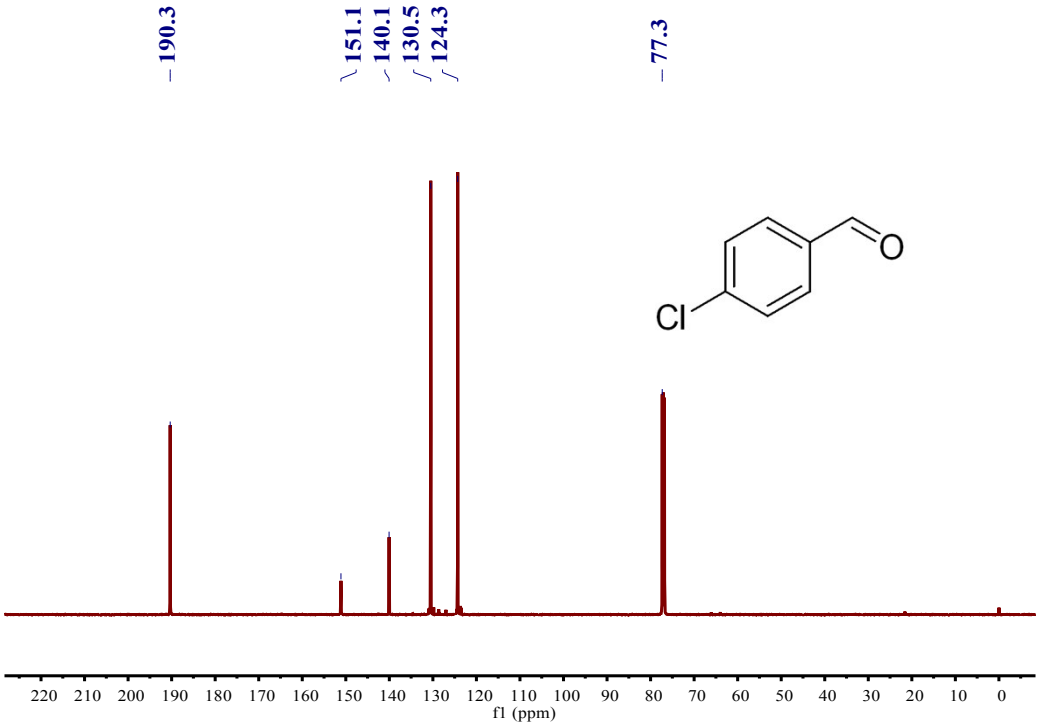

$^{13}$C NMR Spectrum of Compound 4

**Compound 5:** 

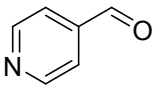
$^{1}$H NMR (500 MHz, $CDCl_3$): δ 9.95 (s, 1H), 7.80 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 190.3, 151.1, 140.1, 130.5, 124.3.



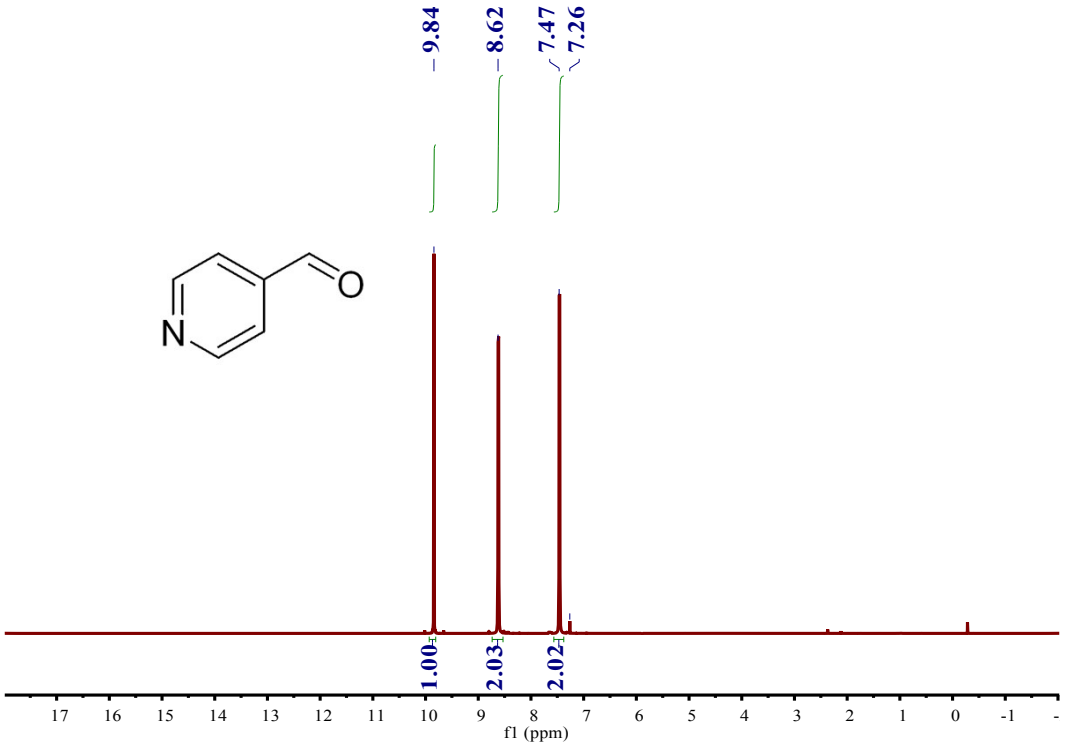

$^{1}$H NMR Spectrum of Compound 5



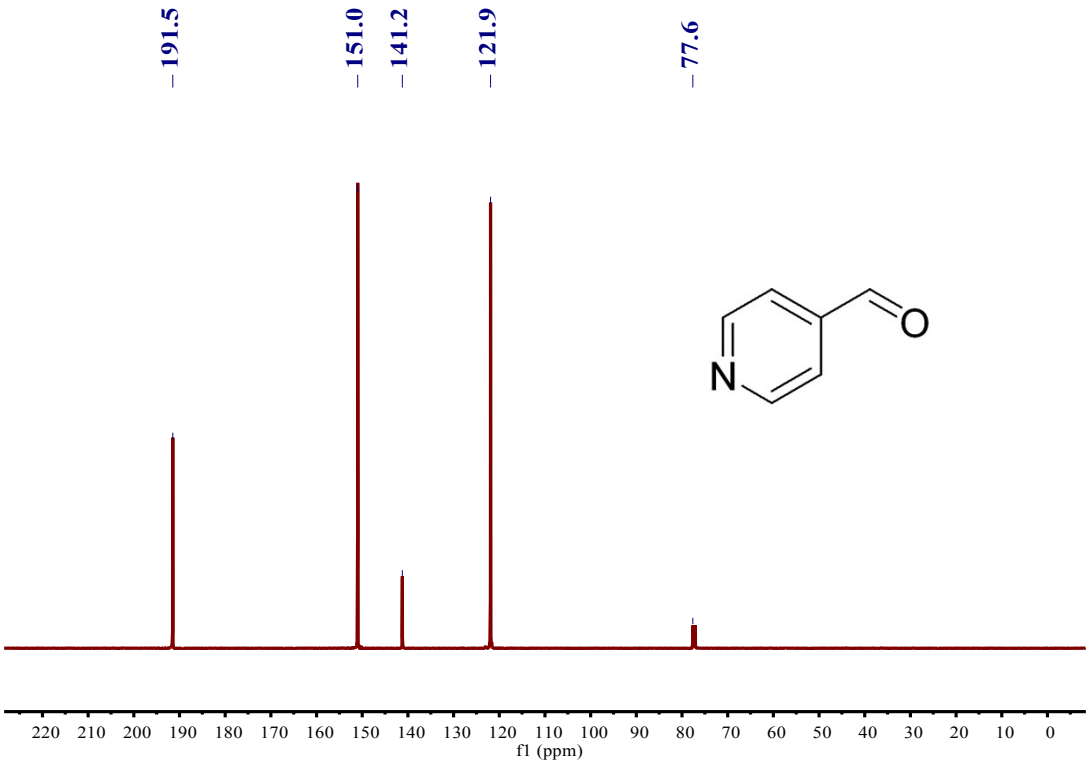

$^{13}$C NMR Spectrum of Compound 5

**Compound 6:** 

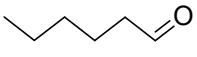
$^{1}$H NMR (500 MHz, $CDCl_3$): δ 9.84 (s, 1H), 8.62 (q, J = 5.9 Hz, 2H), 7.47 (q, J = 5.9 Hz, 2H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 191.5, 151.0, 141.2, 121.9.



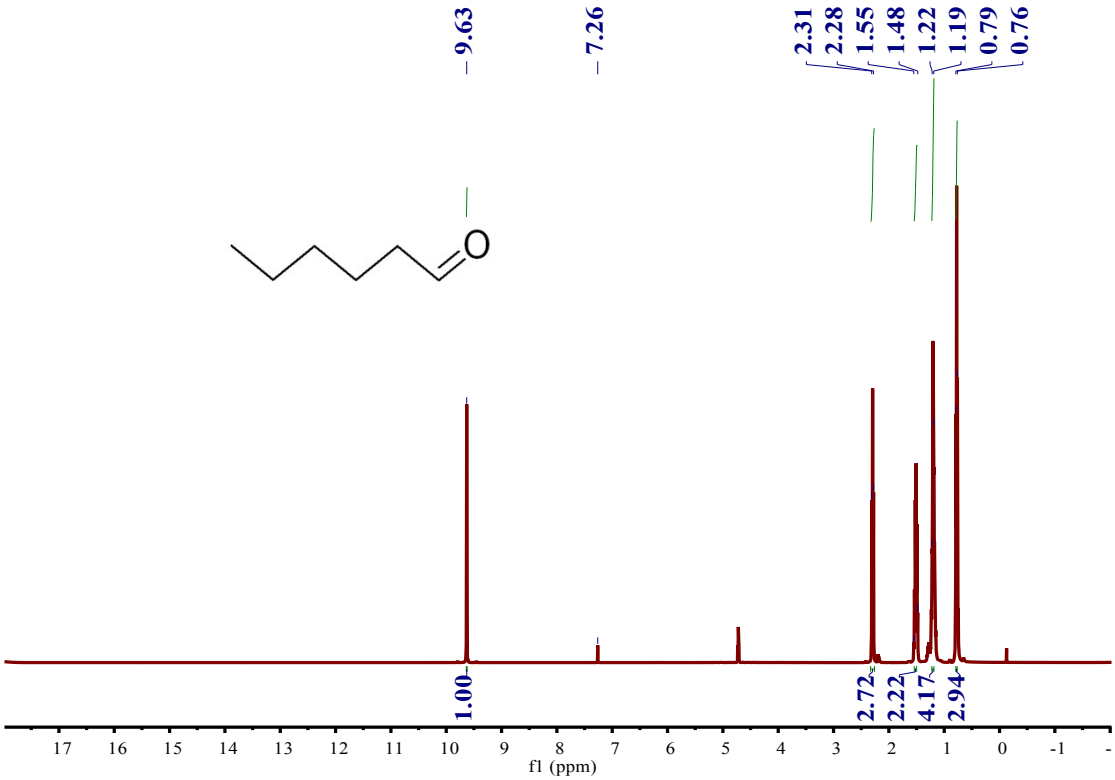

$^{1}$H NMR Spectrum of Compound 6



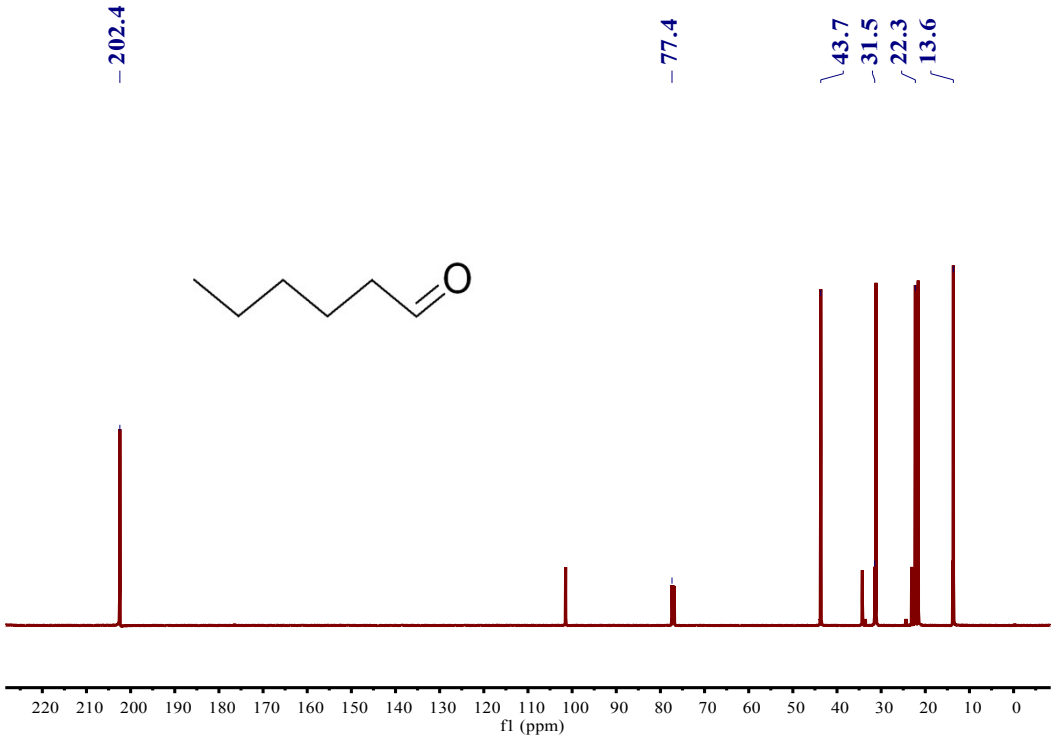

$^{13}$C NMR Spectrum of Compound 6

**Compound 7:** 

$^{1}$H NMR (500 MHz, $CDCl_3$): δ 9.63 (s, 1H), 2.31-2.28 (t, 3H), 1.55-1.48 (quim, 2H), 1.22-1.19(m, 4H), 0.79-0.76 (t, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 202.4, 43.7, 31.5, 22.3, 13.6.



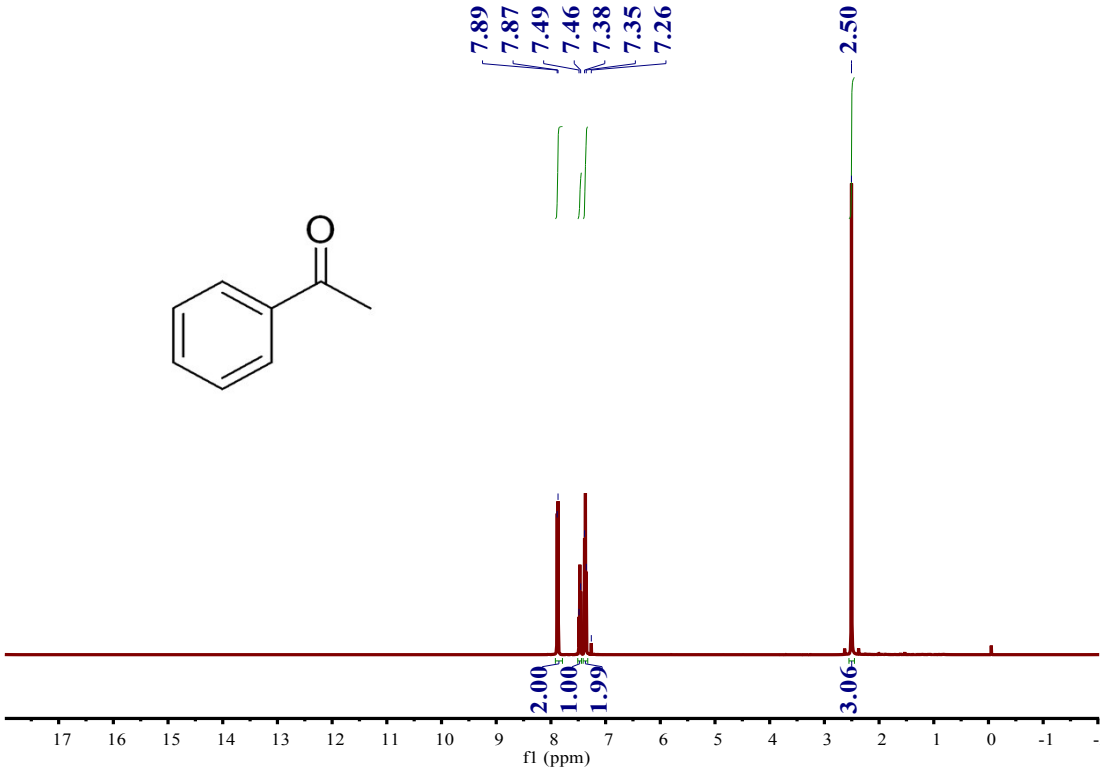

$^{1}$H NMR Spectrum of Compound 7



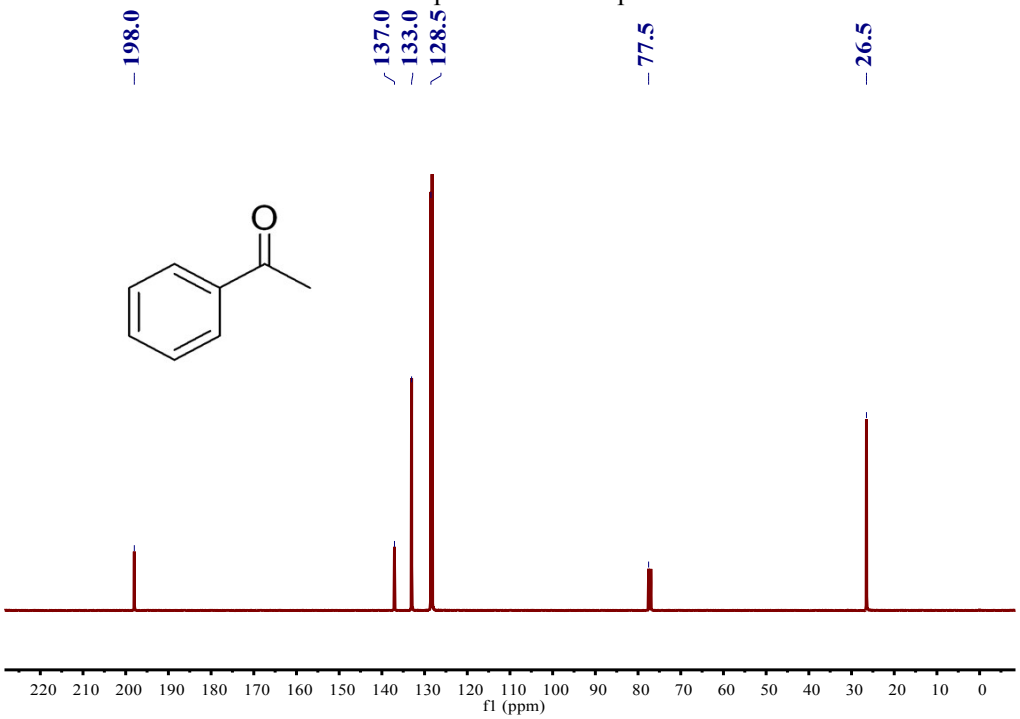

$^{13}$C NMR Spectrum of Compound 7

**Compound 8:**

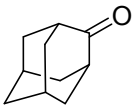
$^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.89-7.87 (m, 2H), 7.49-7.46 (m, 1H), 7.38-7.35 (m, 2H), 2.50 (s, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 198.0, 137.0, 133.0, 128.5, 26.5.



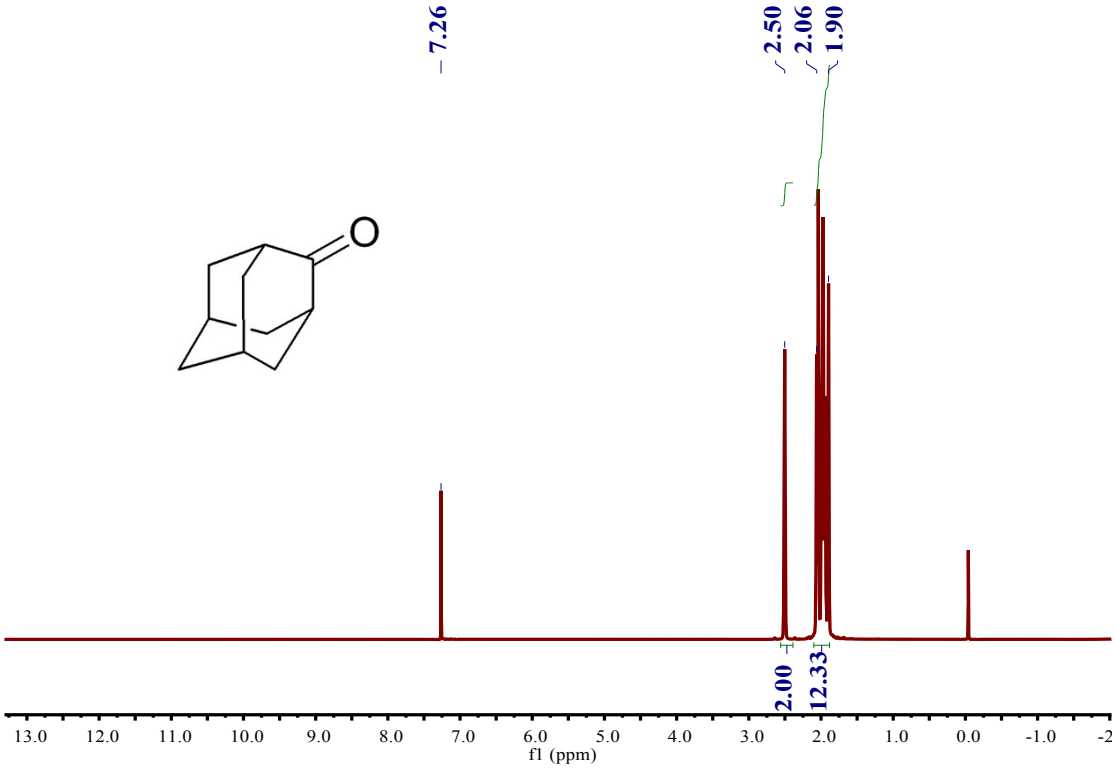

$^{1}$H NMR Spectrum of Compound 8



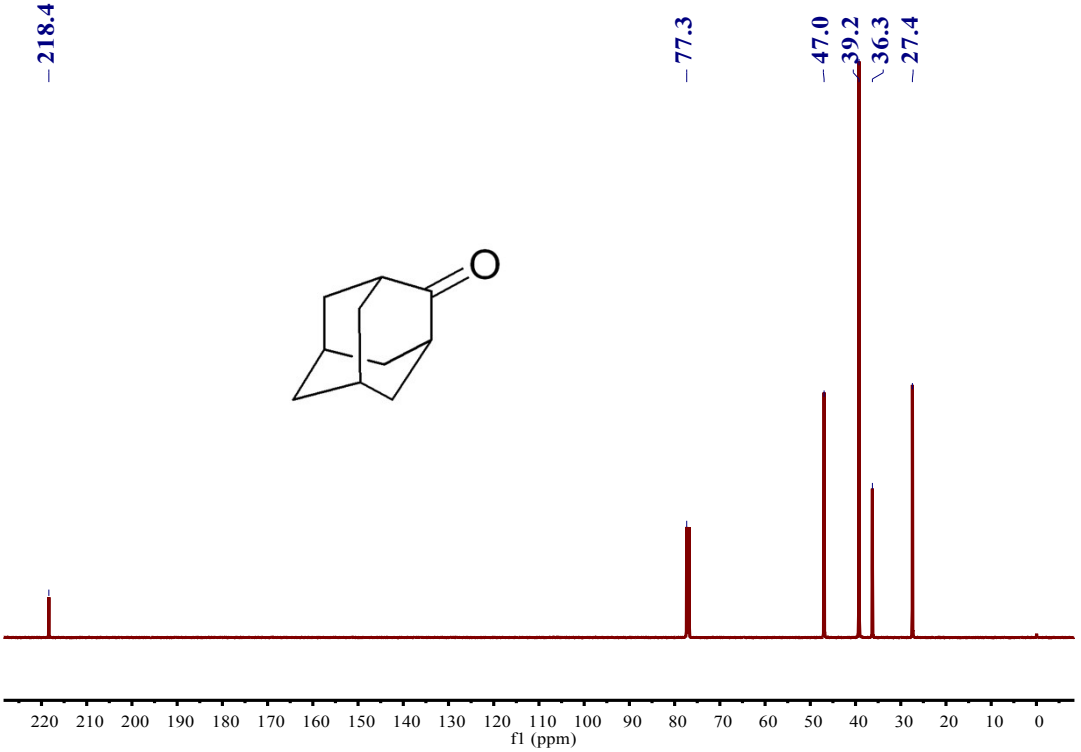

$^{13}$C NMR Spectrum of Compound 8

**Compound 9:** 

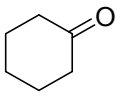
$^{1}$H NMR (500 MHz, $CDCl_3$): δ 2.50 (s, 2H), 2.06-1.90 (m, 12H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 218.4, 47.0, 39.2, 36.3, 27.4.



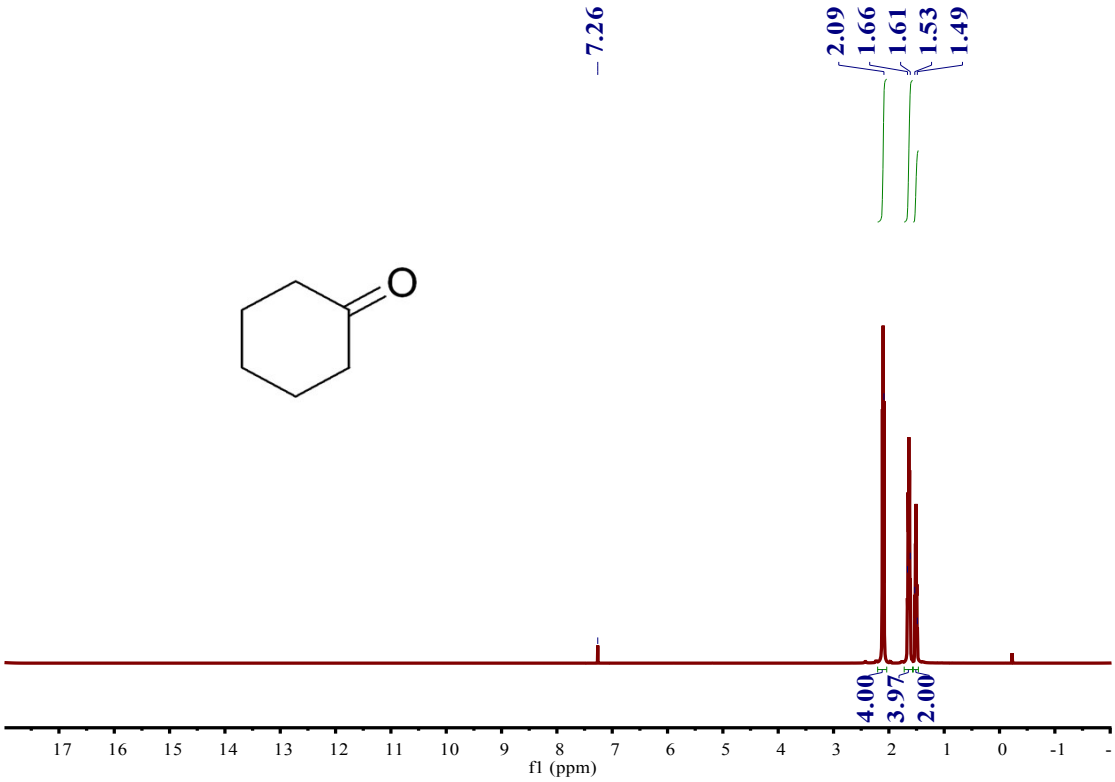

$^{1}$H NMR Spectrum of Compound 9



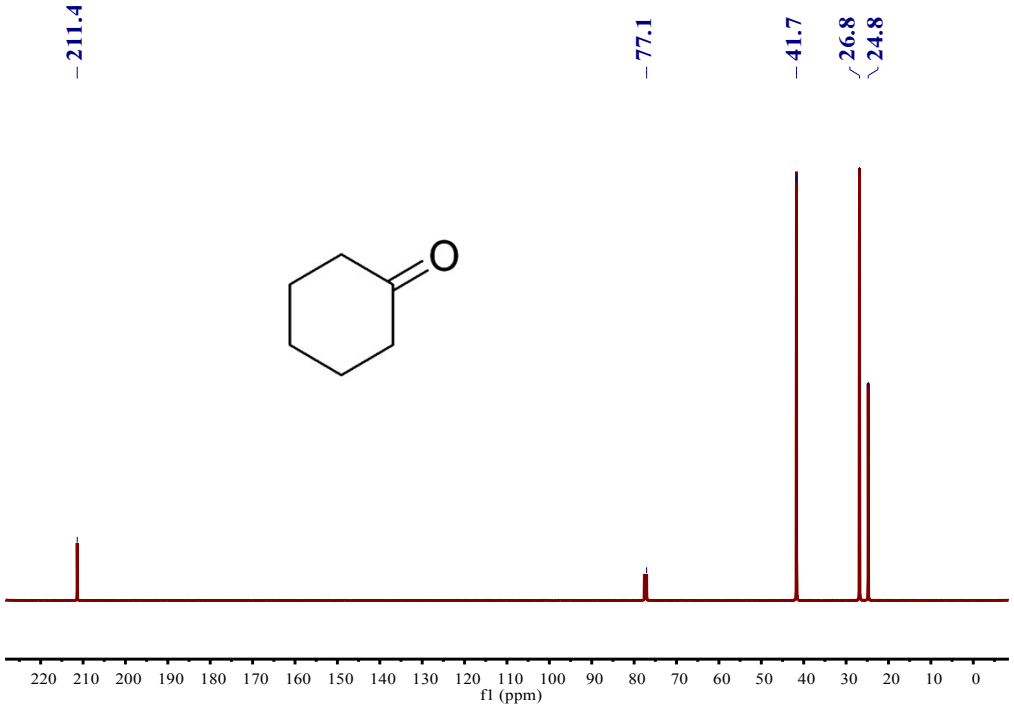

$^{13}$C NMR Spectrum of Compound 9

**Compound 10:** 

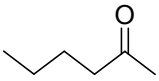
$^{1}$H NMR (500 MHz, $CDCl_3$): δ 2.09 (t, J = 8.0 Hz, 4H), 1.66-1.61 (m, 4H), 1.53-1.49 (m, 2H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 211.4, 41.7, 26.8, 24.8.



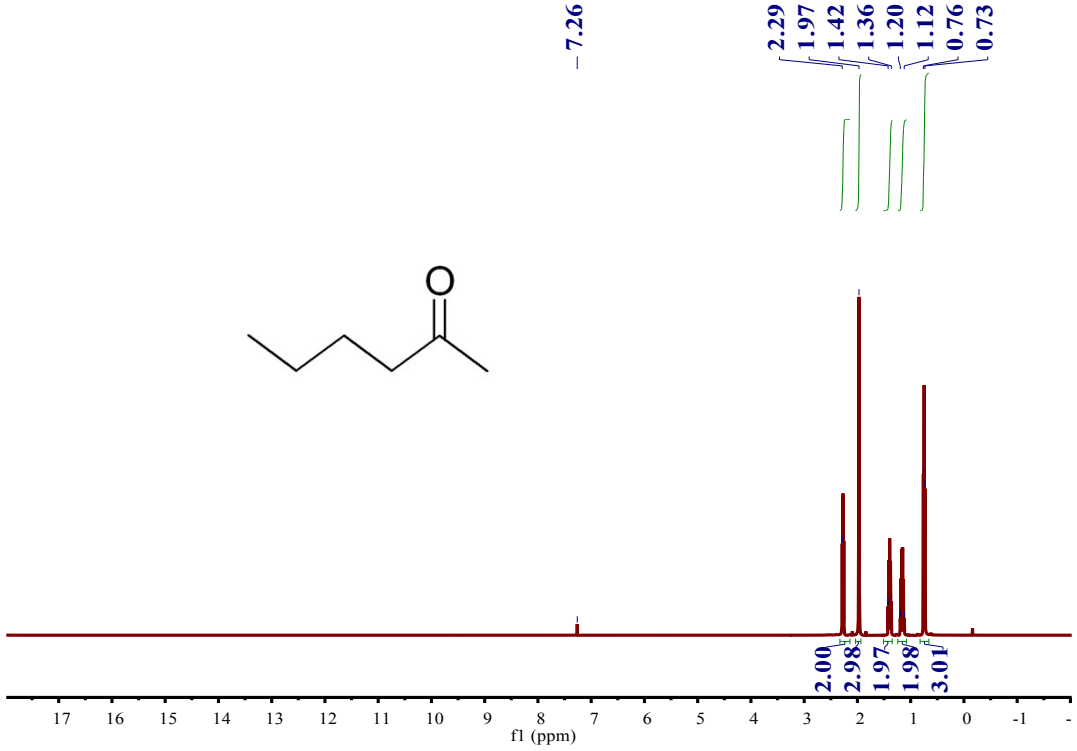

$^{1}$H NMR Spectrum of Compound 10



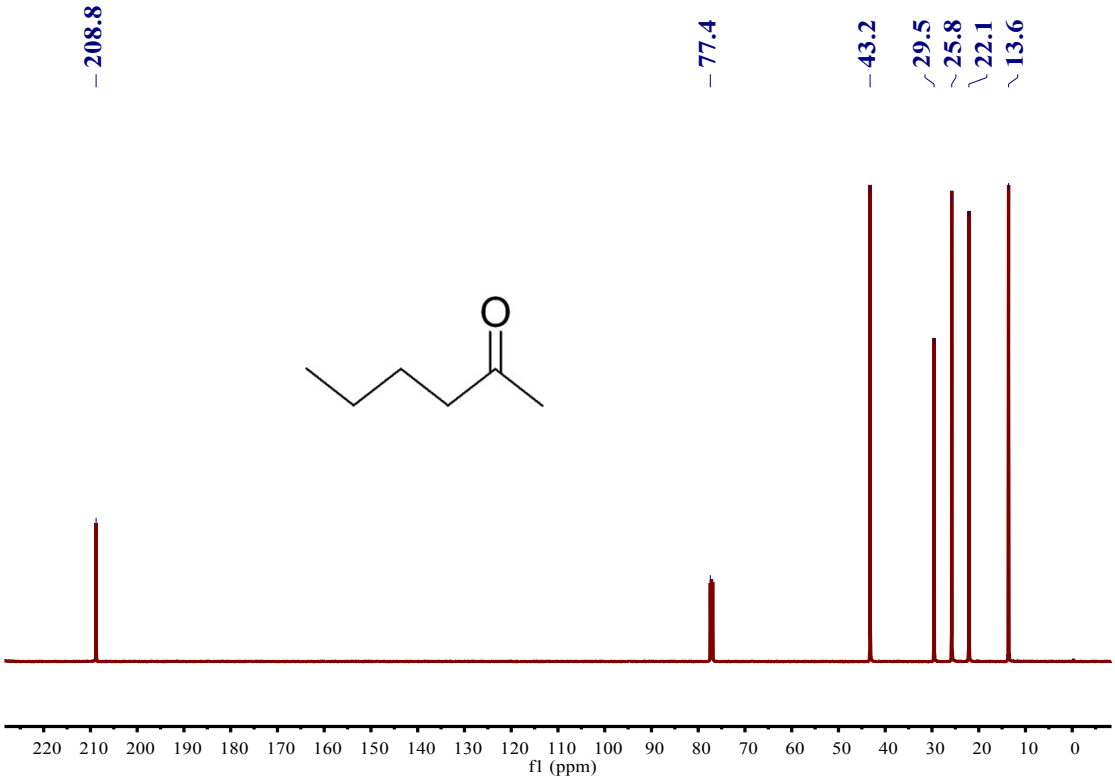

$^{13}$C NMR Spectrum of Compound 10

**Compound 11:** 

$^{1}$H NMR (500 MHz, $CDCl_3$): δ 2.29 (t, J = 7.5 Hz, 2H), 1.97 (s, 3H), 1.42-1.36 (m, 2H), 1.20-1.12 (m, 2H), 0.76-0.73 (m, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$): δ 208.8, 43.2, 29.5, 25.8, 22.1, 13.6.




$^{1}$H NMR Spectrum of Compound 11




$^{13}$C NMR Spectrum of Compound 11