Electronic Supplementary Materials

$NiFe_2O_4$ nanoparticles: An efficient and reusable catalyst for the selective oxidation of benzyl alcohol to benzaldehyde under mild conditions

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Characterization of the product

X-ray diffraction (XRD) study of the dried powder samples was carried out on a Bruker D8 Advance powder X-ray diffractometer using Cu k_α radiation with a wavelength of 0.154 nm. For scanning electron microscopic (SEM) study, a small amount of the dry powder samples were spread on a carbon tape posted on an aluminum stub and then sputter-coated with platinum to minimize the charging effect. The micrographs were then recorded in a field emission scanning electron microscope (FESEM) (Carl Zeiss SUPRA 55 FESEM) at an accelerating voltage of 5 kV. For transmission electron microscopic (TEM) studies, a drop of an aqueous suspension of individual powder sample was cast on a carbon-coated copper grid. The excess solutions were soaked with a tissue paper followed by drying in air. The micrographs were then recorded in a high–resolution JEOL electron microscope (JEM 2100EM) at an accelerating voltage of 200 kV. Dried powder of the samples was subjected to magnetic measurements at room temperature using a Physical Property Measurement System (Quantum Design PPMS-VSM). X-ray photoelectron spectroscopy (XPS) analyses of the dried powder samples were performed in Thermo Fisher Scientific, UK makes ESCALB Xi^+ X-ray photoelectron spectrometer using Al k_α radiations with an incident energy of 1486.61 eV. The instrument was operated at 15 kV and 300 W at ambient temperature under ultrahigh

vacuum. The charging effect on the sample was corrected by setting the binding energy of the carbon (C-1s) at 284.6 eV and this carbon peak was used as a reference position for scaling all the other peaks. Fourier transforms infrared (FTIR) spectra of the powder samples were collected in a Thermo Scientific Nicolet iS5 spectrophotometer in the range of 4000–400 cm^{-1}. The pellets for recording the FTIR spectra were prepared by mixing the powder sample with dried KBr in the weight ratio of 1:100. ^{1}H and ^{13}C NMR spectra were recorded in a JNM ECS 400 MHz NMR spectrophotometer (JEOL) using tetramethylsilane (TMS) as the internal standard. Chemical shift values are expressed in ppm. Coupling constants are expressed in Hertz.

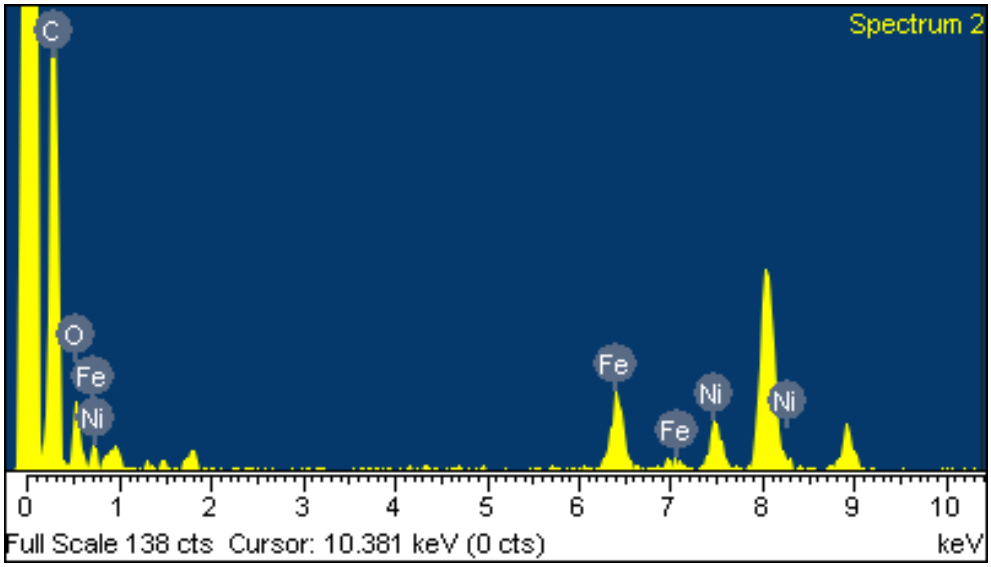


Figure S1. EDX spectrum of $NiFe_2O_4$ NPs recorded from sample $NiFe_2O_4$-4.

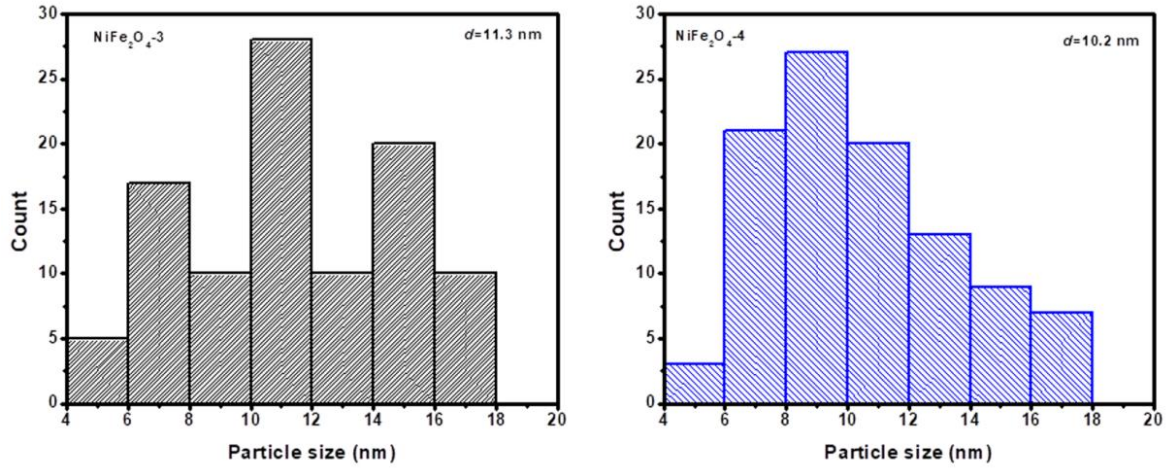


Figure S2. Histograms showing the particle size distribution of $NiFe_2O_4$ NPs in different samples.

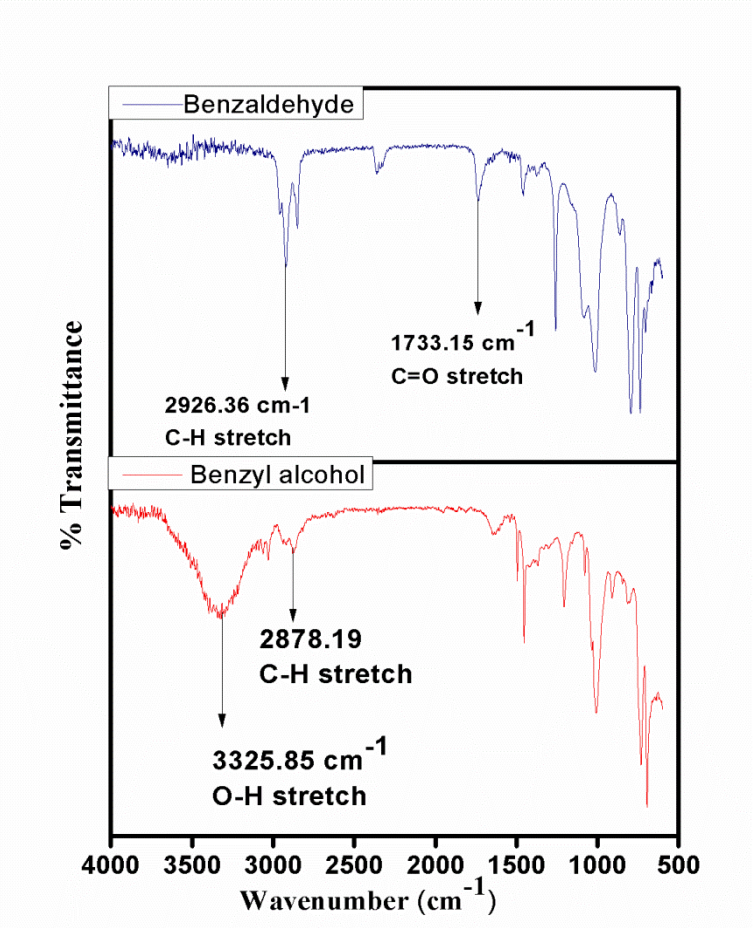
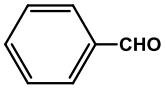


Figure S3. FTIR spectra of benzyl alcohol and its product (benzaldehyde).

Product characterization

Benzaldehyde (Entry 1, Table 3)

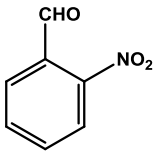


Appearance: Colourless

State: liquid

^{1}H NMR ($CDCl_3$, 400 MHz): δ 10.2 (s, 1H), 7.89-7.87 (d, J=8Hz, 2H), 7.65-7.61 (t, J=8Hz 2H), 7.55-7.51 (t, 2H) ppm

2-Nitro benzaldehyde (Entry 2, Table 3)



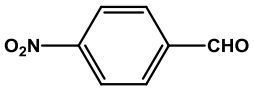
Appearance: white

State: Solid; mp=43-46 °C

^{1}H NMR ($CDCl_3$, 500 MHz): δ 10.404 (s, 1H), 8.112-8.095 (t, J=4.5 Hz 1H), 7.944-7.927 (m, 1H), 7.803-7.732 (m, 2H) ppm

^{13}C NMR ($CDCl_3$, 125 MHz): δ 188.125, 149.925, 134.056, 133.677, 131.229, 129.598, 124.462 ppm

4-Nitro benzaldehyde (Entry 4, Table 3)



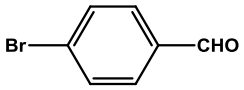
Appearance: Pale yellow

State: Solid; mp = 104-106 °C

^{1}H NMR ($CDCl_3$, 500 MHz): δ 10.096 (s, 1H), 8.342-8.325 (2, J=4.5 Hz t), 8.027-8.001 (2, m) ppm

^{13}C NMR ($CDCl_3$, 125 MHz): δ 190.375, 151.220, 140.121, 130.573, 124.403 ppm

4-Bromo benzaldehyde (Entry 6, Table 3)



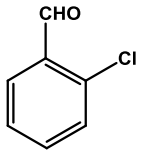
Appearance**:** White

State: solid; mp=57 °C

^{1}H NMR (CDCl3, 400 MHz): δ 9.97 (s, 1H), 7.75-7.73 (d, J=8 Hz, 2H), 7.69-7.67 (d, J=8 Hz, 2H) ppm

^{13}C NMR ($CDCl_3$, 100 MHz): 191.26, 135.20, 132.67, 131.12, 129.86 ppm

2-Chloro benzaldehyde (Entry 7, Table 3)

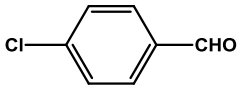


Appearance**:** Yellow coloured

State: Liquid

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.872 (s, 1H), 7.835-7.818 (m, 1H), 7.55-7.52 (m, 1H), 7.46-7.40 (m, 1H), 7.38-7.36 (d, 1H) ppm.

4-Chloro benzaldehyde (Entry 8, Table 3)



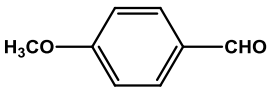
Appearance**:** Pale yellow

State: Powder; mp=45 °C

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.93 (s, 1H), 7.78-7.76 (d, J=8 Hz, 2H), 7.47-7.45 (d, J=8 Hz, 2H) ppm

^{13}C NMR ($CDCl_3$, 100 MHz): 190.97, 141.02, 134.85, 131.03, 129.54 ppm

4-Methoxy benzaldehyde (Entry 9, Table 3)



Appearance: Light yellow

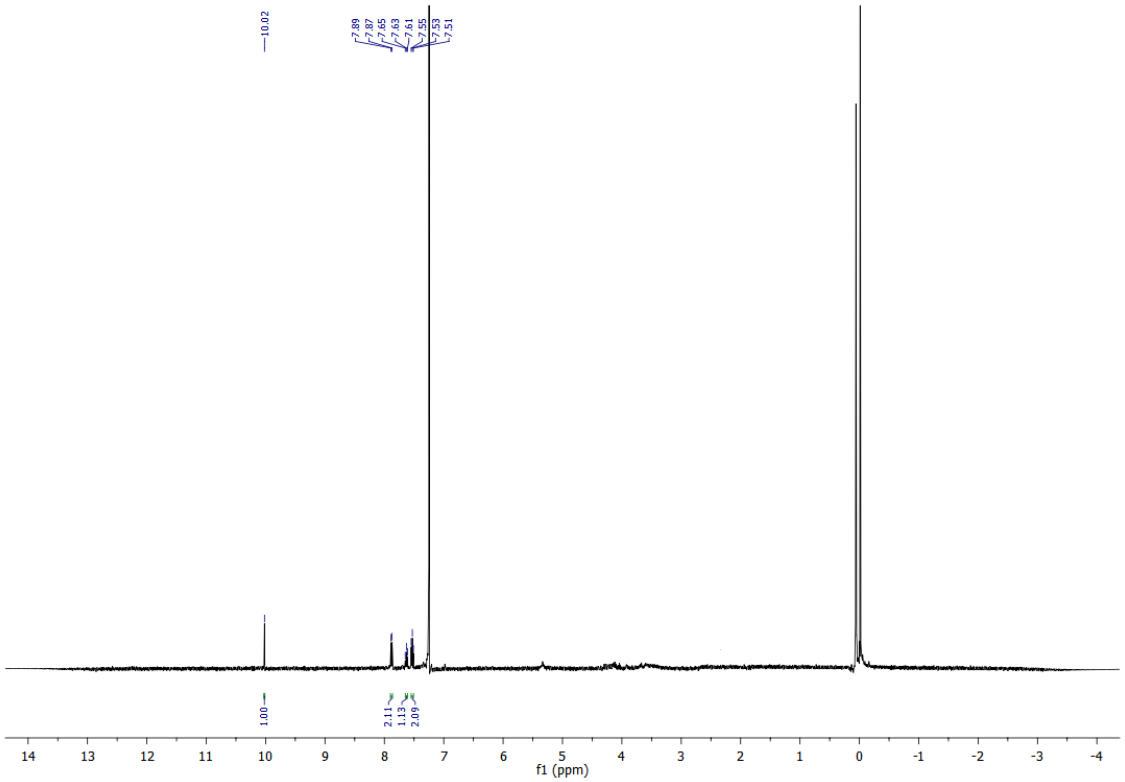
State: liquid

^{1}H NMR ($CDCl_3$, 500 MHz): δ 9.87 (s, 1H), 7.835-7.818 (t, J=4.25 Hz, 2H), 7.000-6.983 (t, J=4.25 Hz, 2H), 3.877 (s, 3H) ppm

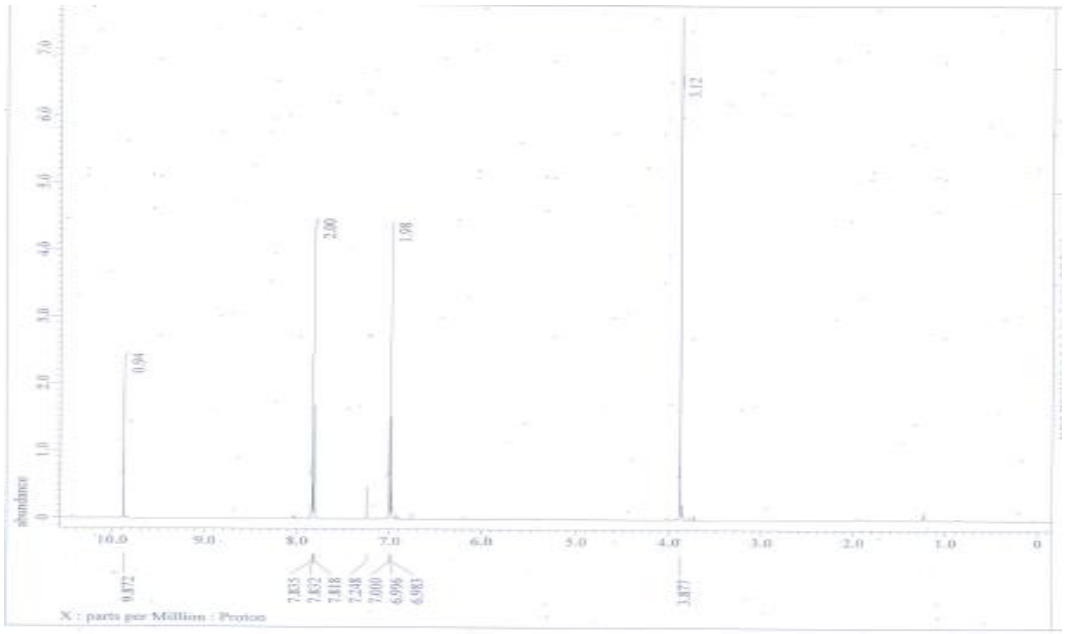
^{13}C NMR ($CDCl_3$, 125 MHz): δ 191.10, 141.02, 134.85, 131.03, 129.54 ppm

^{1}H and ^{13}C NMR of selected isolated products

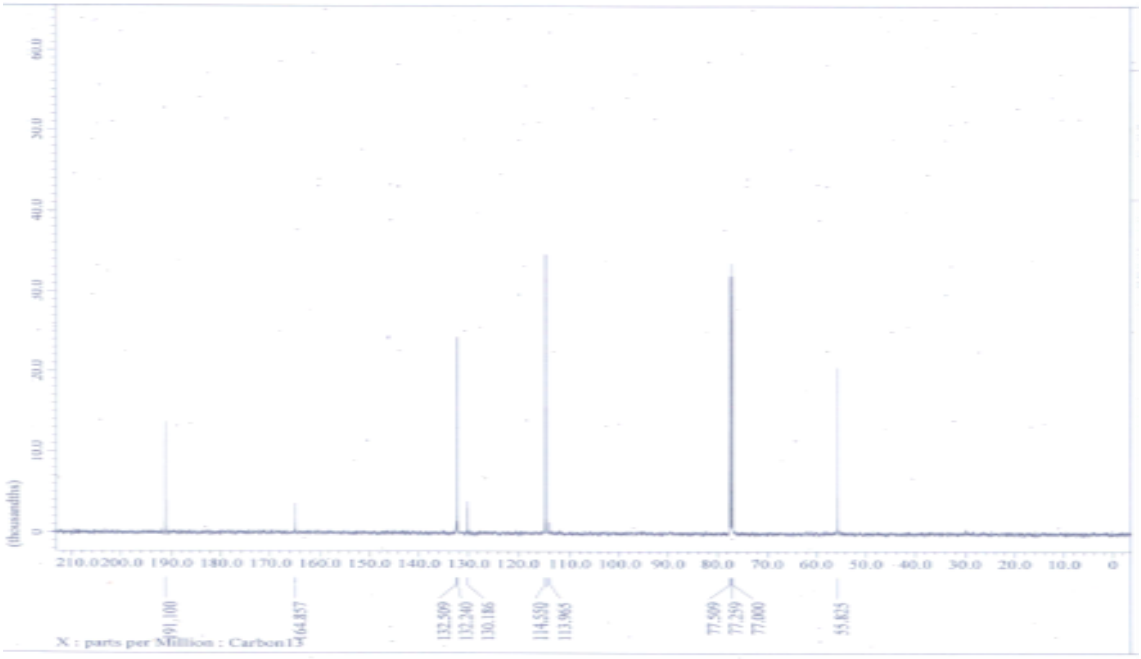
^{1}H NMR of benzaldehyde



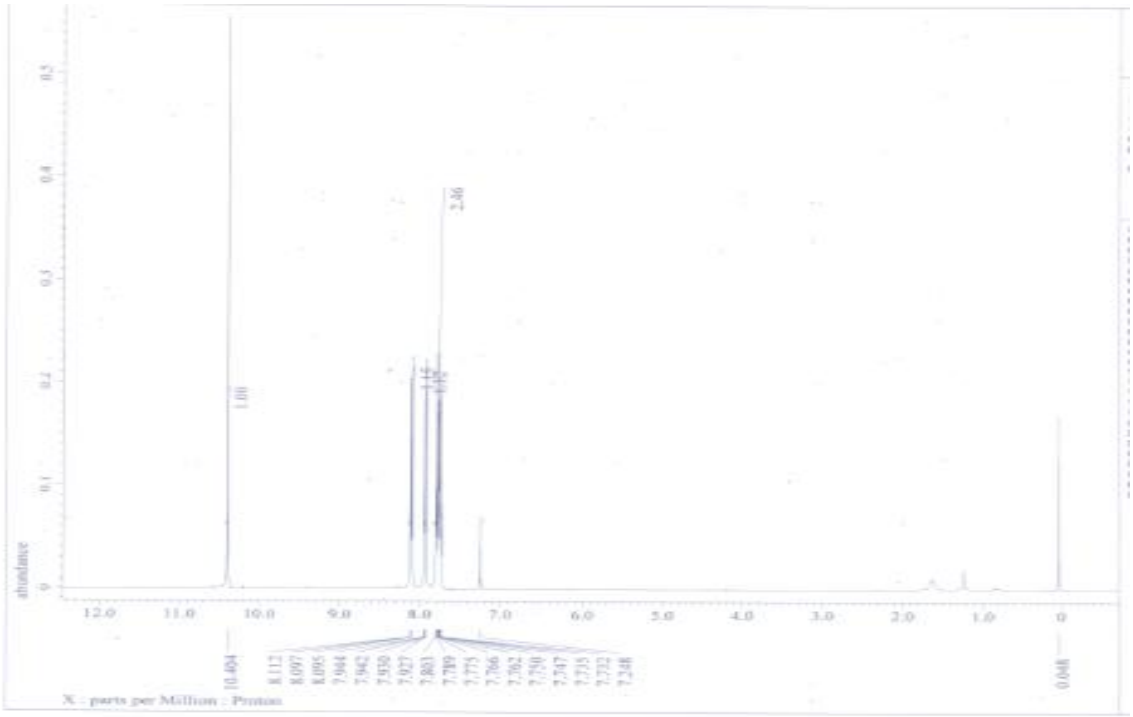
^{1}H NMR spectrum of 4-methoxy benzaldehyde



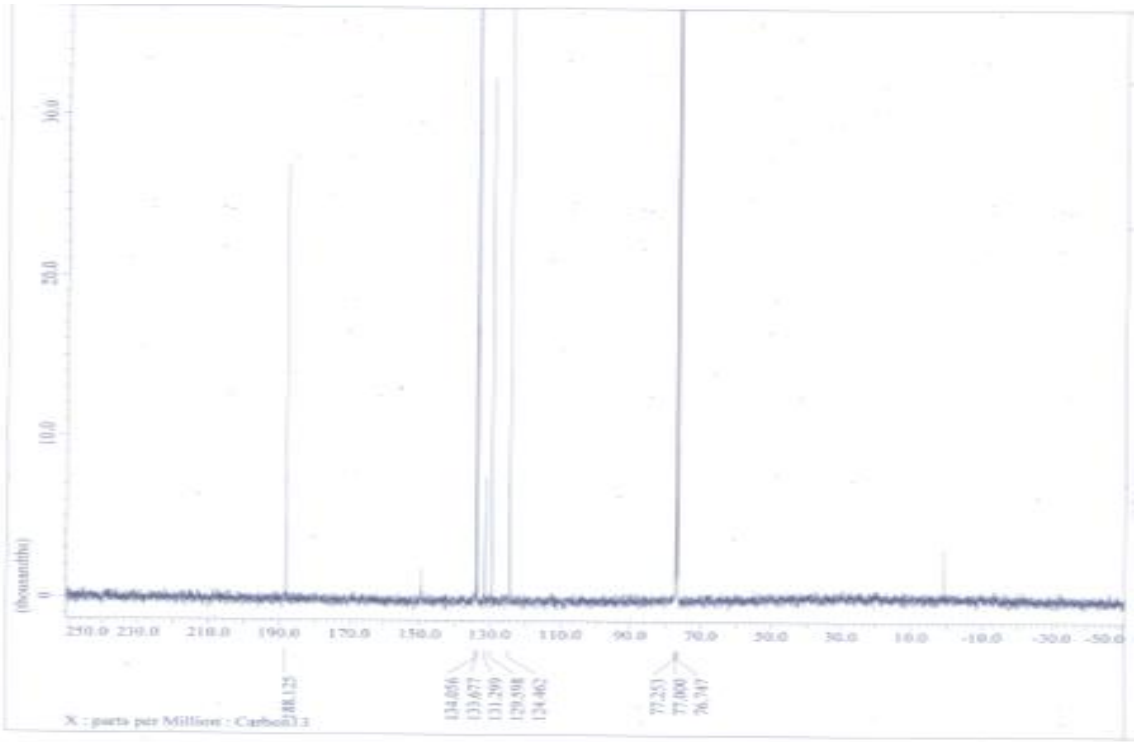
^{13}C NMR spectrum of 4-methoxy benzaldehyde



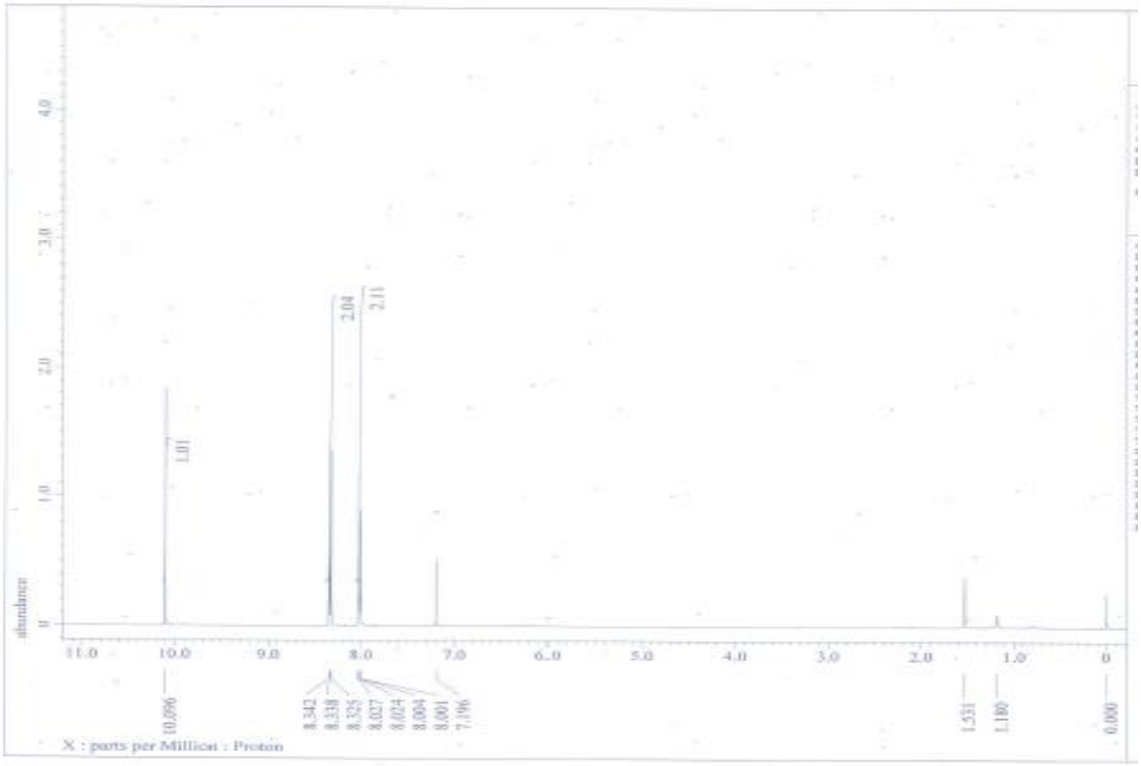
^{1}H NMR spectrum of 2-nitro benzaldehyde



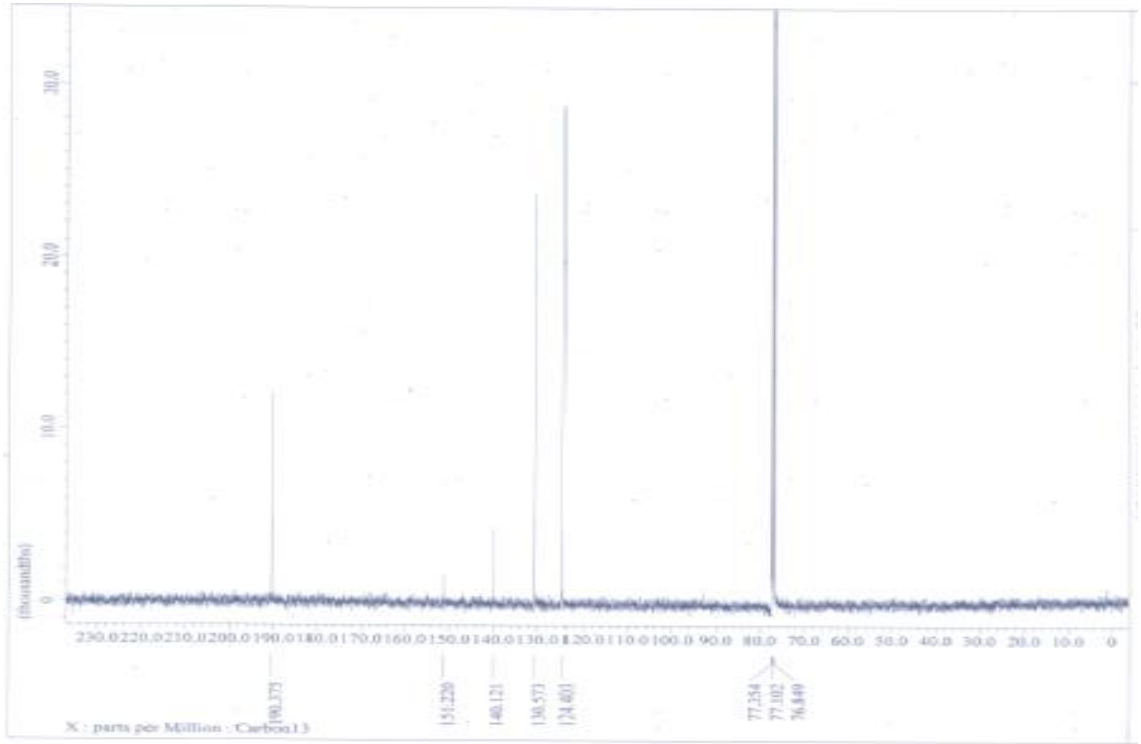
^{13}C NMR spectrum of 2-nitro benzaldehyde



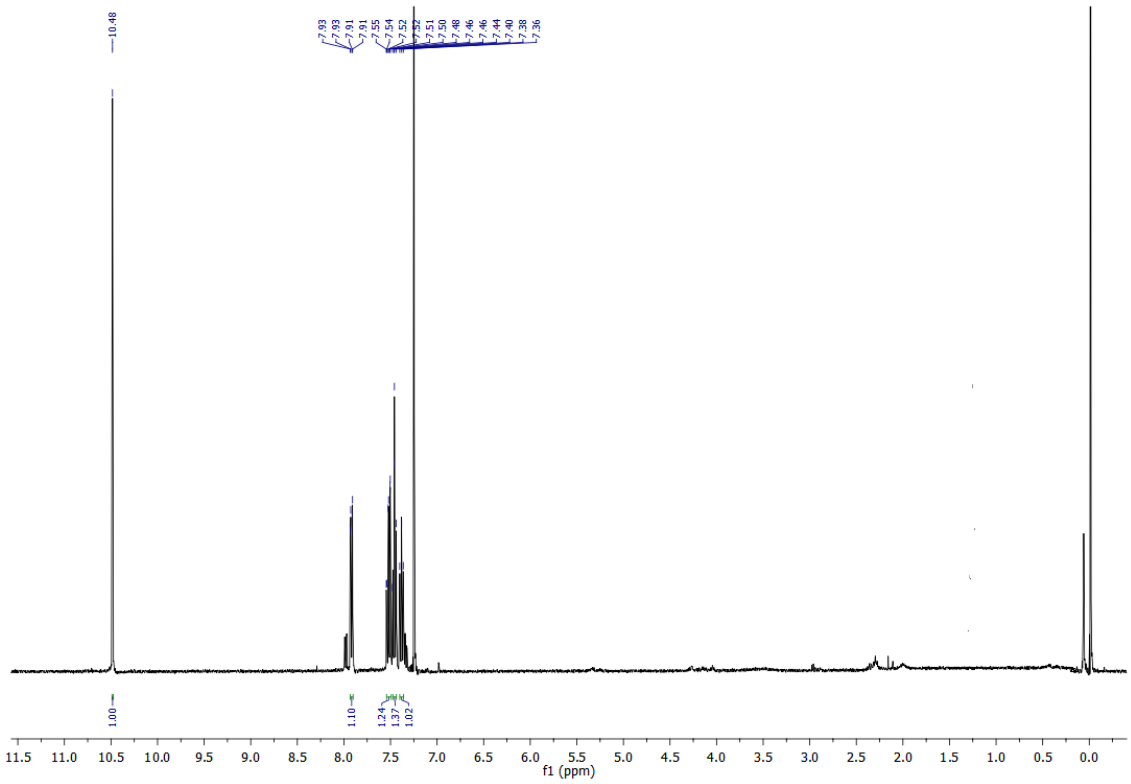
^{1}H NMR spectrum of 4-nitro benzaldehyde



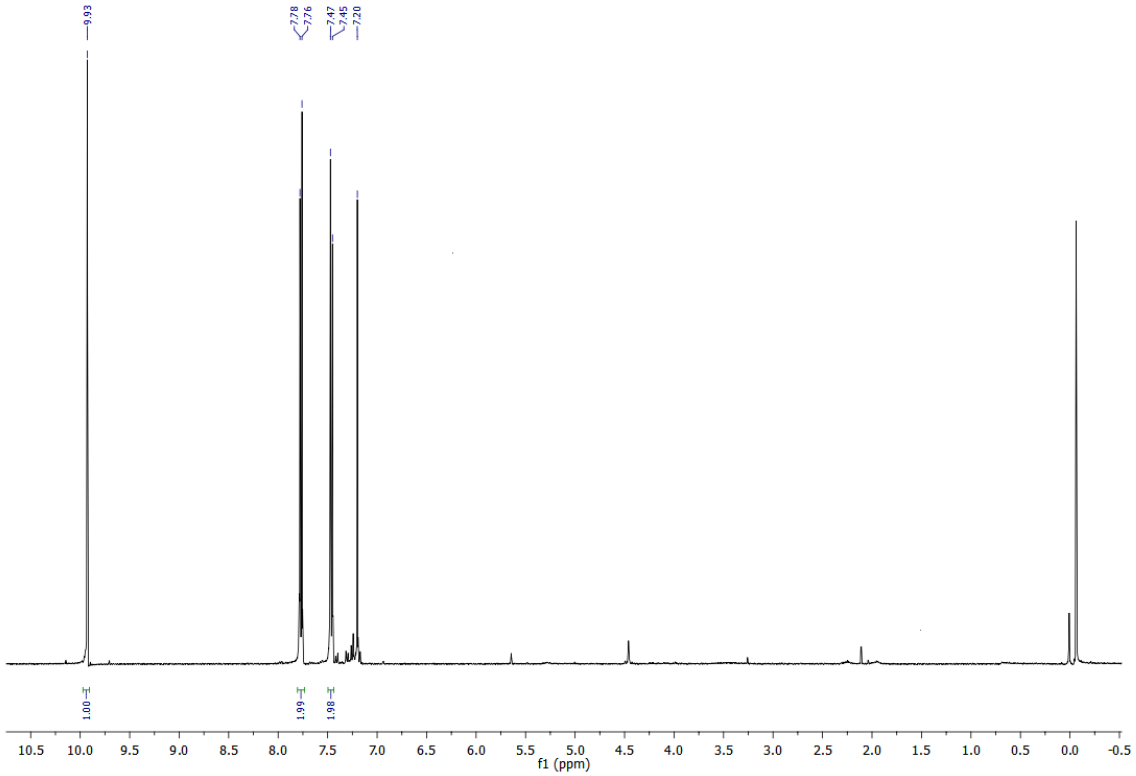
^{13}C NMR spectrum of 4-nitro benzaldehyde



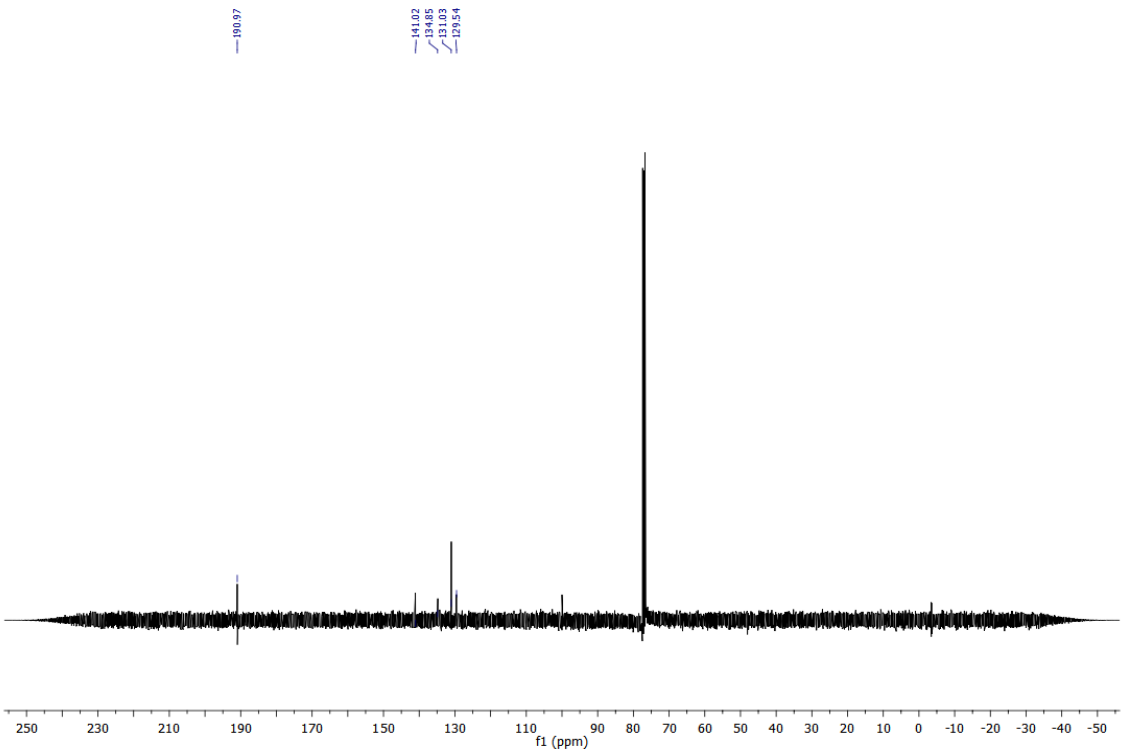
^{1}H NMR spectrum of 2-Chloro benzaldehyde



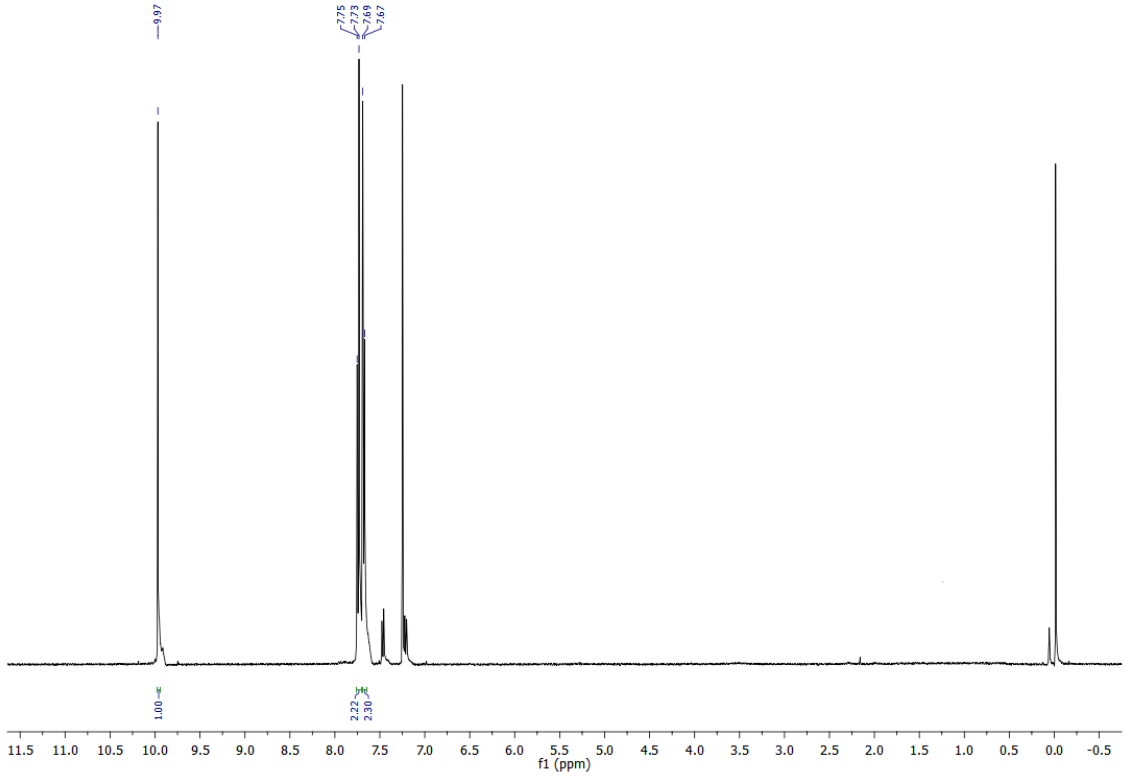
^{1}H NMR spectrum of 4-Chloro benzaldehyde



^{13}C NMR spectrum of 4-Chloro benzaldehyde



^{1}H NMR spectrum of 4-Bromo benzaldehyde



^{13}C NMR spectrum of 4-Bromo benzaldehyde