Supporting Information

Anti-Markovnikov primary alcohols via terminal epoxide hydrogenation by Y-doped Al_2O_3-supported CoNi nanoparticles

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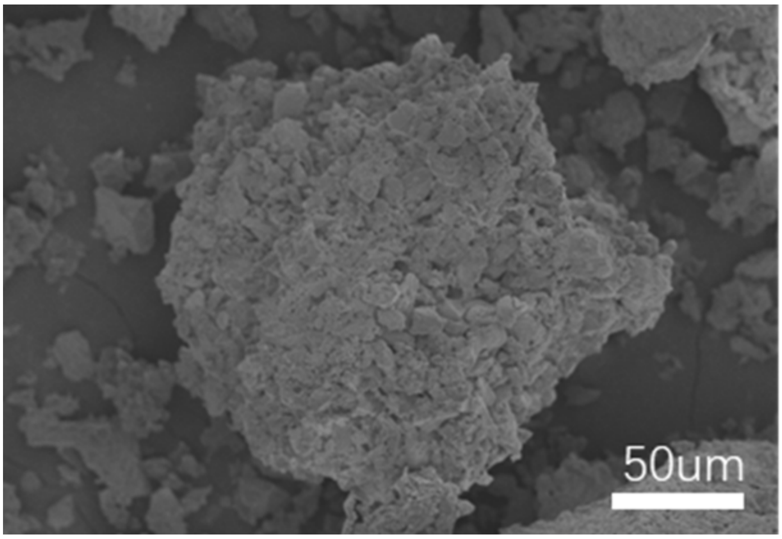


Figure S1 SEM images of NiCo/Y-Al_2O_3 catalyst

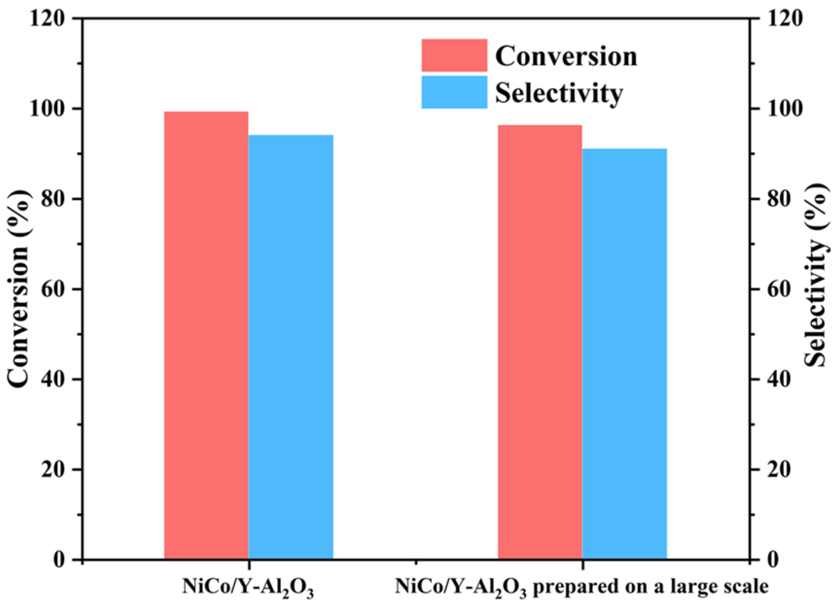


Figure S2. Enhance the catalytic performance of the catalyst

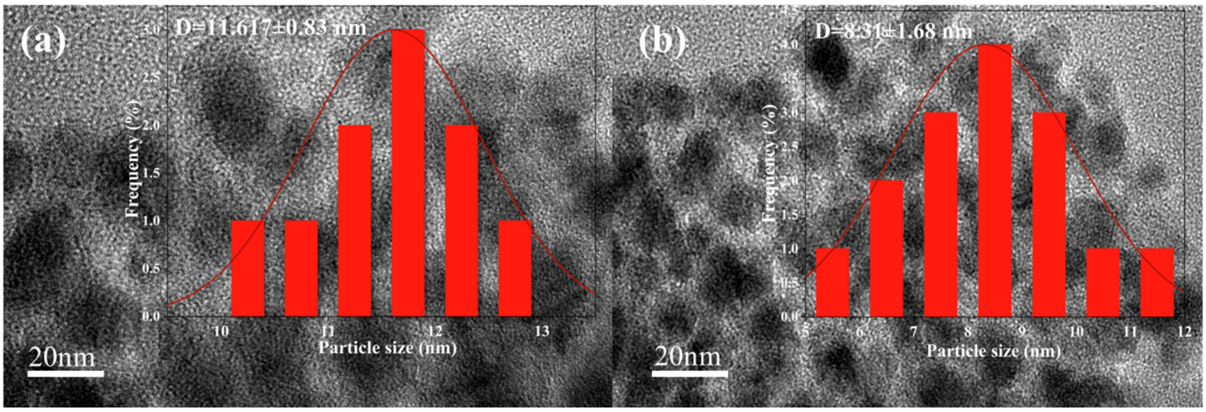


Figure S3. TEM images of (a) Ni/Y-Al_2O_3 (b) NiCo/Y-Al_2O_3

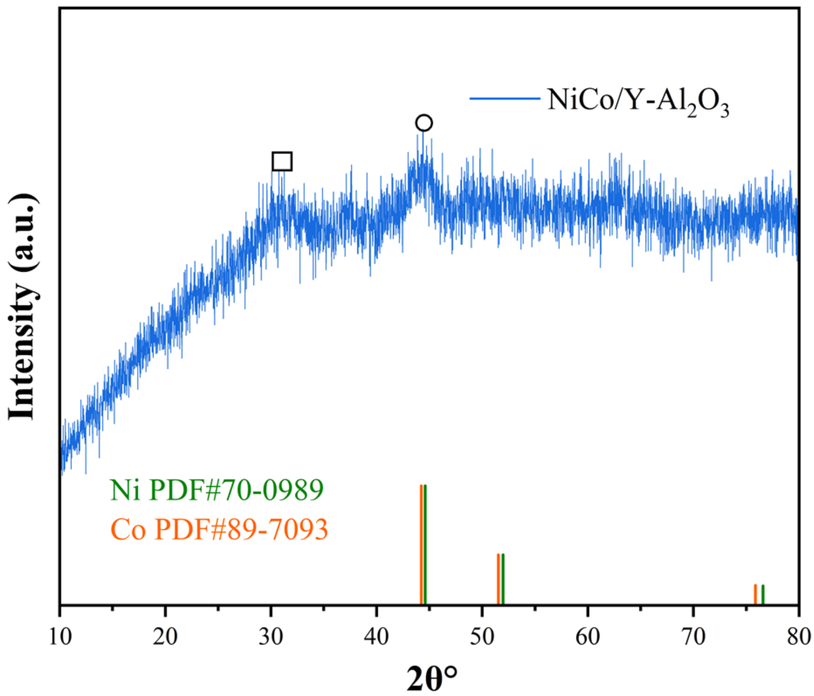


Figure S4. XRD patterns of NiCo/Y-Al_2O_3: □ Indicates amorphous aluminum oxide, ○ Indicates NiCo

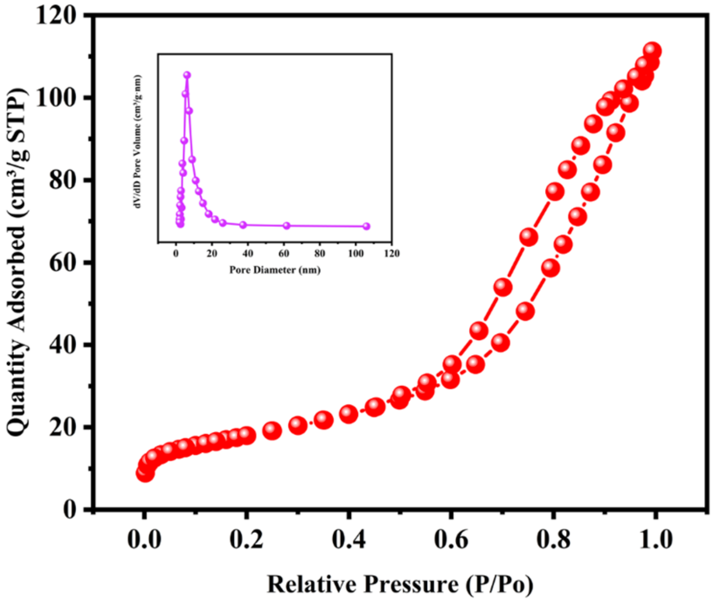


Figure S5. Nitrogen adsorption/desorption isotherm of NiCo/Y-Al_2O_3 (inset showing pore size distribution)

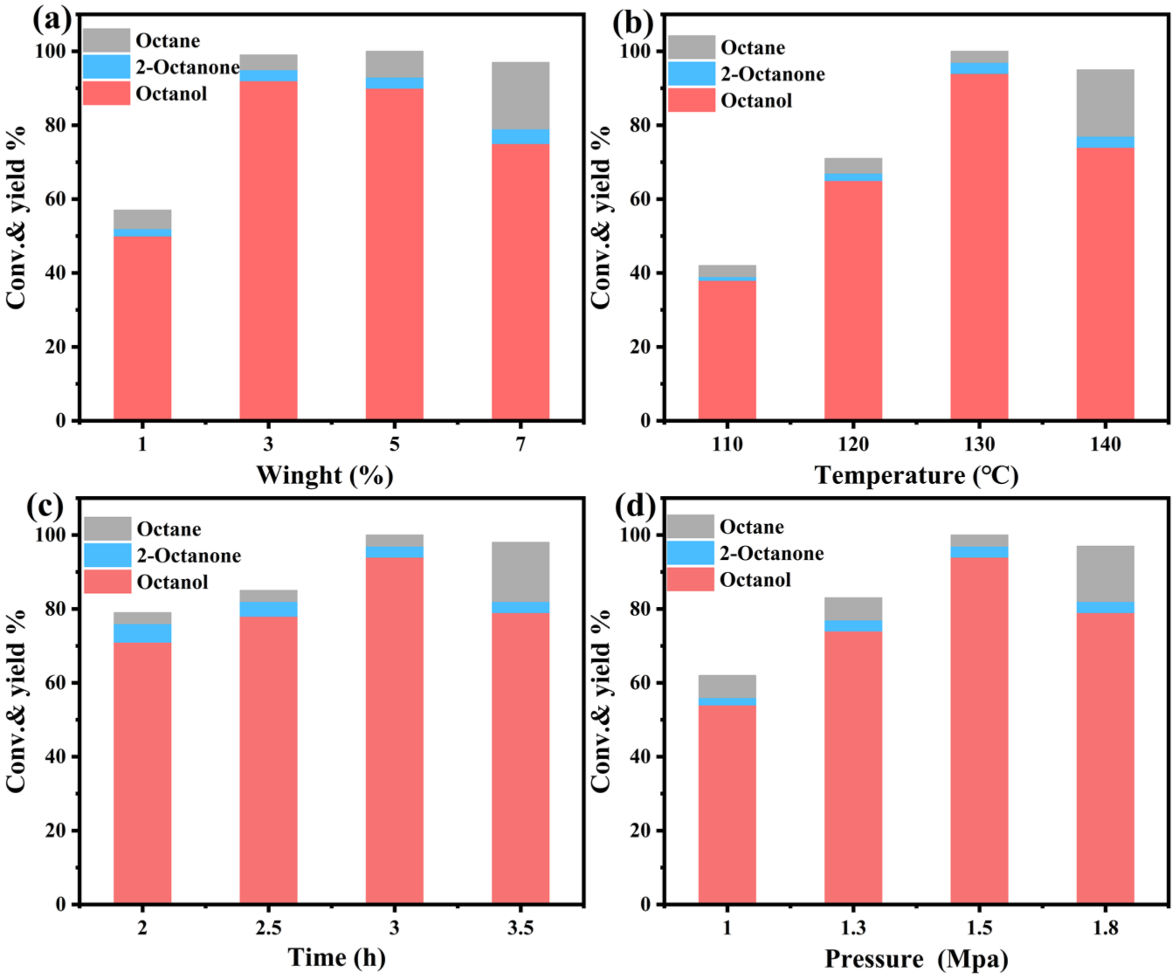


Figure S6. (a) The influence of catalyst dosage (b) The influence of reaction temperature (c) The influence of reaction time (d) The influence of reaction pressure

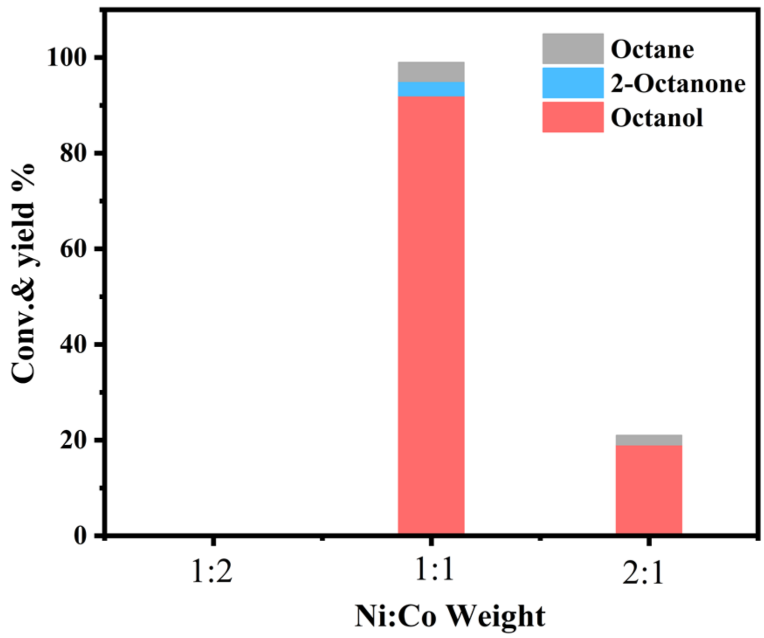


Figure S7. Different NiCo comparisons

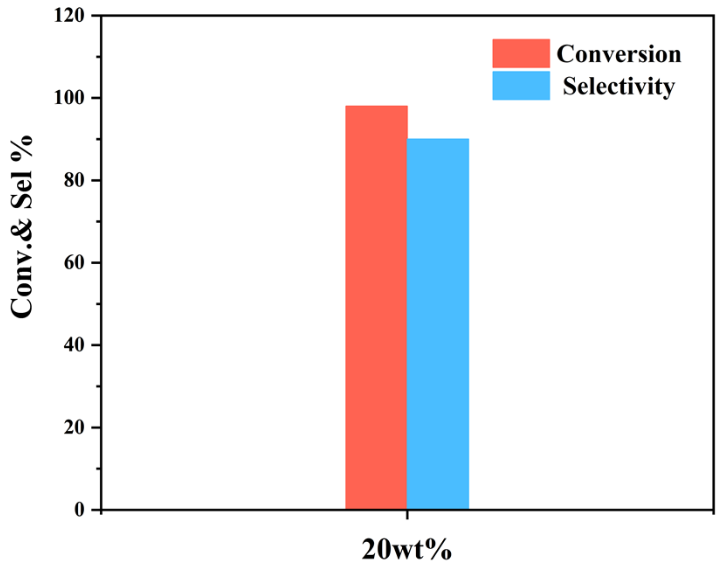


Figure S8. Reaction result of 25.6 g (200 mmol) 1,2-epoxyoctane in 100 mL THF at 20 wt% concentration, 130°C, 3 h, 1.5 MPa

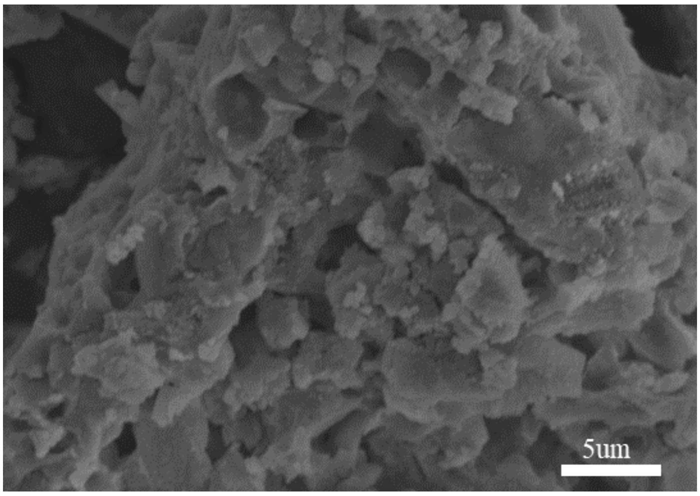


Figure S9. SEM image of NiCo/Y-Al_2O_3 after catalysis

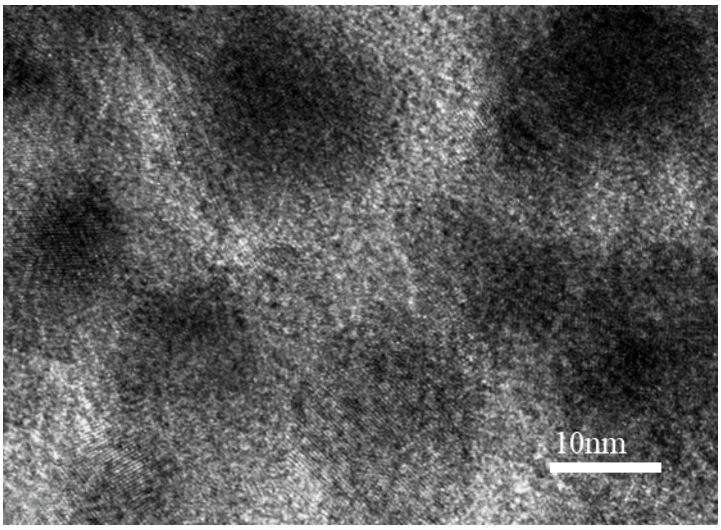


Figure S10. TEM image of NiCo/Y-Al_2O_3 after catalysis

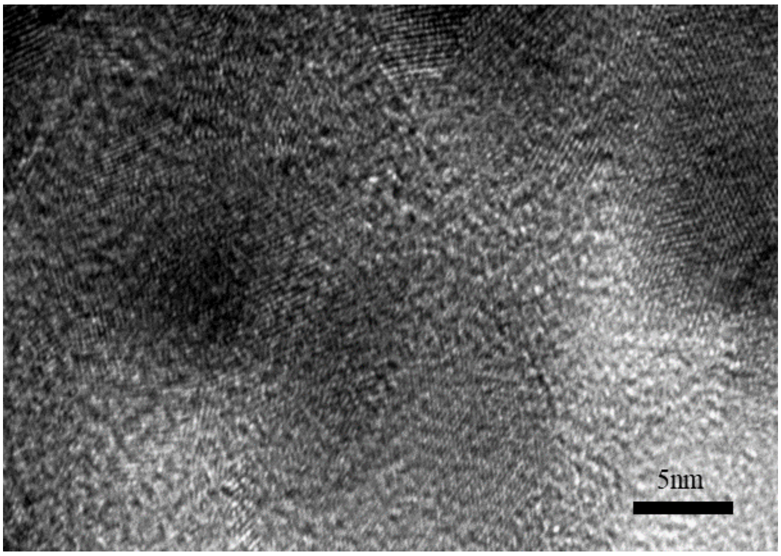


Figure S11. HR-TEM image of NiCo/Y-Al_2O_3 after catalysis

Table S1. ICP-OES characterization of Ni/Al_2O_3, $NiCo/Al_2O_3$, $NiCo/Y\text{-}Al_2O_3$.

catalyst	Ni/Co Actual Load (%)
Ni/Al_2O_3	4.3241
$NiCo/Al_2O_3$	4.4057/4.3531
$NiCo/Y\text{-}Al_2O_3$	4.3472/4.3752

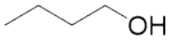
Table S2. Base amount determined by CO_2-TPD

catalyst	Weak base center mmol/g	Strong base site mmol/g	Strong/weak base	Total base content mmol/g
Ni/Al_2O_3	0.006	0.261	43.5	0.267
$NiCo/Al_2O_3$	0.009	0.143	15.8	0.152
$NiCo/Y\text{-}Al_2O_3$	0.062	0.133	2.14	0.195

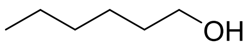
Table S3. Acid amount determined by NH_3-TPD

catalyst	Weak acid center mmol/g	Strong acid center mmol/g	Strong /weak acid	Total acid content mmol/g
Ni/Al_2O_3	0.142	0.240	1.69	0.382
$NiCo/Al_2O_3$	0.133	0.374	2.81	0.507
$NiCo/Y\text{-}Al_2O_3$	0.080	0.183	2.28	0.263

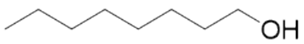
Characterization data



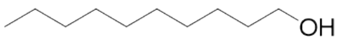
1-Butanol (1.76g 88%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.51 (t, *J* = 6.7 Hz, 2H), 2.68 (s, 1H), 1.44 (dt, *J* = 14.9, 6.8 Hz, 2H), 1.27 (dq, *J* = 14.5, 7.3 Hz, 2H), 0.83 (t, *J* = 7.4 Hz, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 62.51 (s), 34.78 (s), 18.87 (s), 13.79 (s). ESI-MS: m/z =75 $[M+1]^+$."



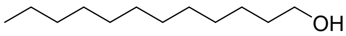
1-hexanol (1.90g 95%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.51 (t, *J* = 6.7 Hz, 2H), 2.47 (s, 1H), 1.54 – 1.40 (m, 2H), 1.31 – 1.13 (m, 6H), 0.80 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 62.86 (s), 32.69 (s), 31.63 (s), 25.41 (s), 22.60 (s), 13.96 (s). ESI-MS: m/z =103 $[M+1]^+$."



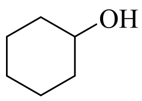
1-Octanol (1.88g 94%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.53 (t, *J* = 6.7 Hz, 2H), 2.20 (s, 1H), 1.46 (dd, *J* = 14.2, 7.0 Hz, 2H), 1.32 – 1.11 (m, 9H), 0.80 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 62.88 (s), 32.74 (s), 31.80 (s), 29.39 (s), 29.26 (s), 25.75 (s), 22.62 (s), 14.03 (s). ESI-MS: m/z =131 $[M+1]^+$."



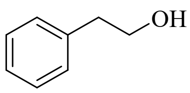
1-Decanol (1.86g 93%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.54 (t, *J* = 6.7 Hz, 2H), 2.00 (s, 1H), 1.53 – 1.42 (m, 2H), 1.31 – 1.12 (m, 13H), 0.81 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 62.92 (s), 32.76 (s), 31.89 (s), 29.62 (s), 29.56 (s), 29.44 (s), 29.31 (s), 25.75 (s), 22.65 (s), 14.05 (s). ESI-MS: m/z =159 $[M+1]^+$."



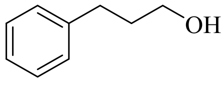
1-Dodecanol (1.80g 90%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.55 (t, *J* = 6.7 Hz, 2H), 1.84 (s, 1H), 1.54 – 1.44 (m, 2H), 1.34 – 1.13 (m, 16H), 0.81 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 62.94 (s), 32.77 (s), 31.91 (s), 29.80 – 29.24 (m), 25.76 (s), 22.67 (s), 14.07 (s). ESI-MS: m/z =187 $[M+1]^+$."



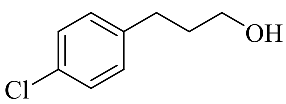
Cyclohexanol (1.84g 92%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.54 – 3.42 (m, 1H), 2.41 (s, 1H), 1.78 (dt, *J* = 9.1, 5.0 Hz, 2H), 1.68 – 1.56 (m, 2H), 1.49 – 1.38 (m, 1H), 1.24 – 0.97 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 70.22 (s), 35.48 (s), 25.46 (s), 24.14 (s). ESI-MS: m/z =101 $[M+1]^+$."



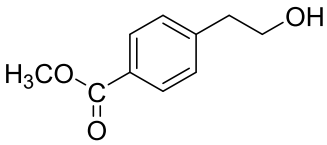
Phenethyl alcohol (1.92g 96%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.13 (m, 5H), 3.76 (t, *J* = 6.7 Hz, 2H), 2.80 (t, *J* = 6.7 Hz, 2H), 2.29 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.58 (s), 128.83 (d, *J* = 47.5 Hz), 126.48 (s), 63.66 (s), 39.22 (s). ESI-MS: m/z =123 $[M+1]^+$."



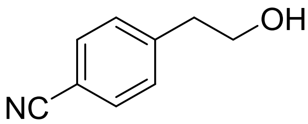
3-Phenyl-1-propanol (1.86g 93%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.09 (m, 5H), 3.61 (t, *J* = 6.5 Hz, 2H), 2.75 – 2.58 (m, 2H), 2.44 (s, 1H), 1.92 – 1.78 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.96 (s), 128.48 (d, *J* = 4.0 Hz), 125.91 (s), 62.11 (s), 34.25 (s), 32.15 (s). ESI-MS: m/z =137 $[M+1]^+$."



4-Chlorophenethyl alcohol (1.80g 90%)^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.05 (m, 4H), 3.75 (t, *J* = 6.6 Hz, 2H), 2.77 (t, *J* = 6.6 Hz, 2H), 2.38 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.12 (s), 132.25 (s), 130.37 (s), 128.64 (s), 63.37 (s), 38.45 (s). ESI-MS: m/z =157 $[M+1]^+$."



methyl 4-(2-hydroxyethyl)benzoate(1.74g 87%) ^{1}H NMR (400 MHz, CDCl3) δ 7.93 (d, J = 8.3 Hz, 2H), 7.26 (d, J = 8.2 Hz, 2H), 5.28 (s, 1H), 3.87 (s, 3H), 3.82 (t, J = 6.7 Hz, 2H), 2.88 (d, J = 6.7 Hz, 2H). ^{13}C NMR (101 MHz, CDCl3) δ 167.20 (s), 144.52 (s), 129.71 (s), 129.03 (s), 128.11 (s), 62.97 (s), 52.03 (s), 39.10 (s).



4-(2-hydroxyethyl)benzonitrile(1.70g 85%) ^{1}H NMR (400 MHz, CDCl3) δ 7.57 (d, J = 8.2 Hz, 2H), 7.35 (d, J = 8.1 Hz, 2H), 3.85 (t, J = 6.4 Hz, 2H), 2.91 (t, J = 6.5 Hz, 2H), 2.37 (s, 1H). ^{13}C NMR (101 MHz, CDCl3) δ 144.91 (s), 132.21 (s), 129.90 (s), 119.00 (s), 109.98 (s), 62.71 (s), 39.14 (s).

NMR Spectra

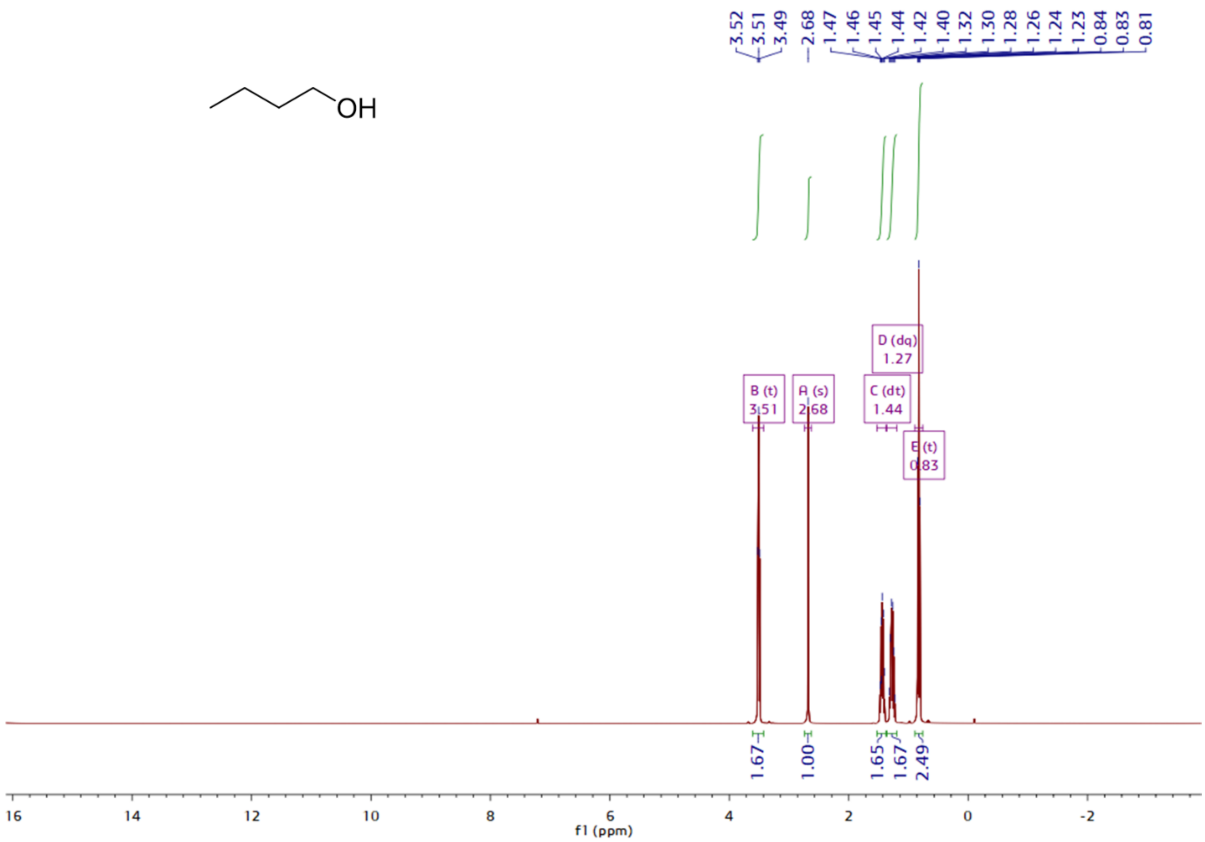


Fig.1 ^{1}HNMR

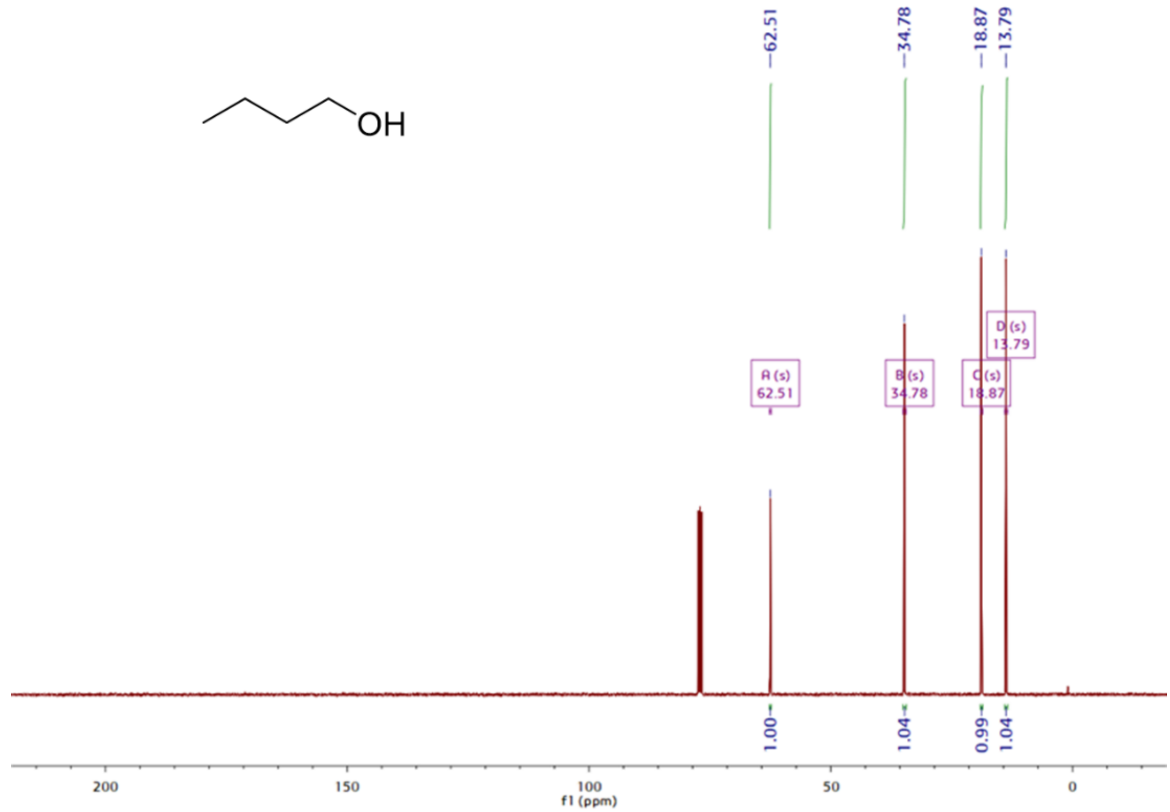


Fig.2 ^{13}C NMR

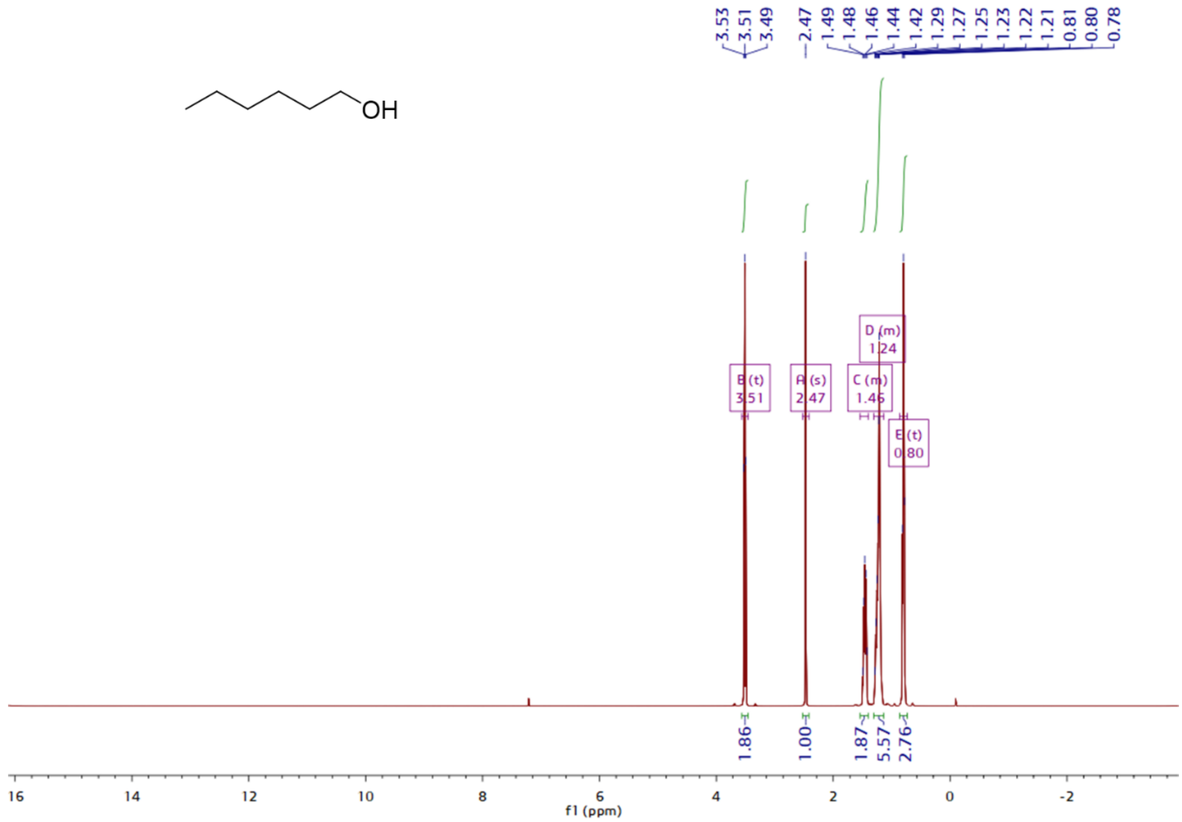


Fig.3 ^{1}H NMR

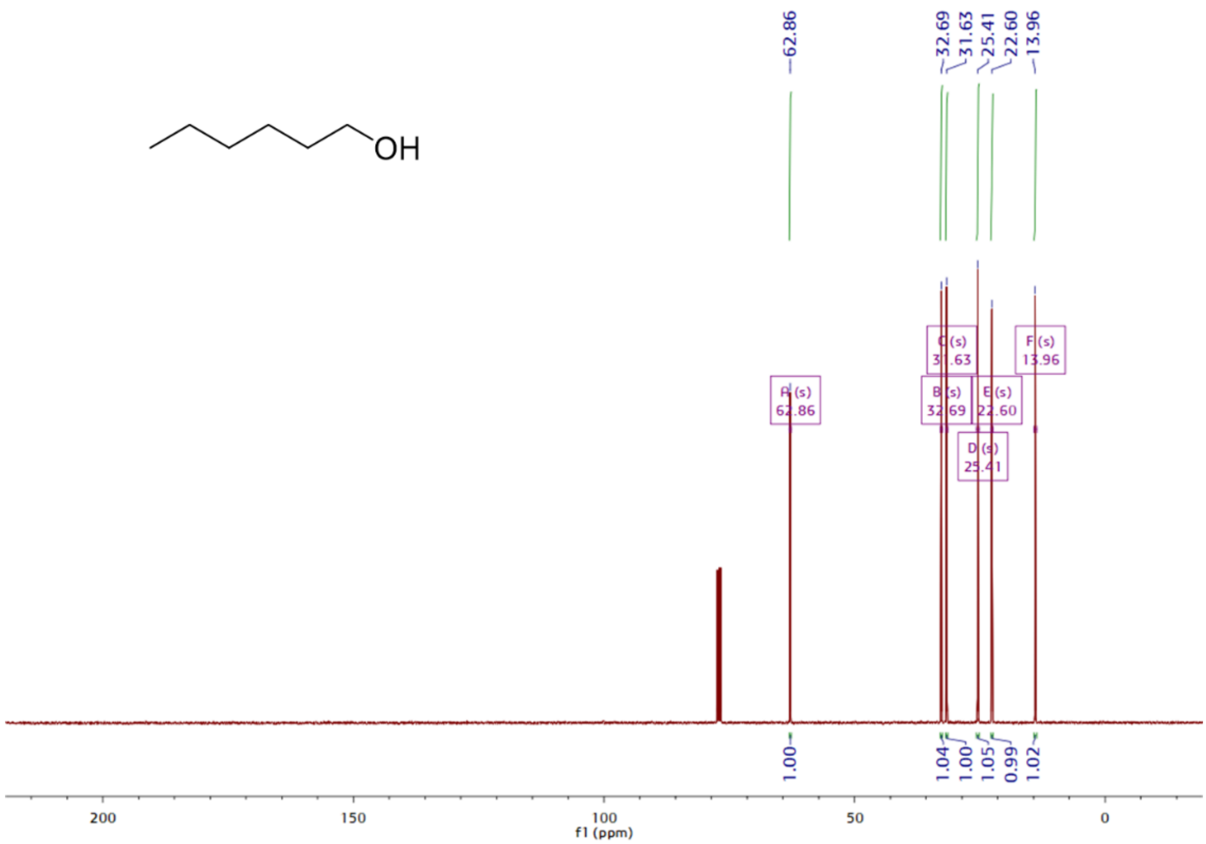


Fig.4 ^{13}C NMR

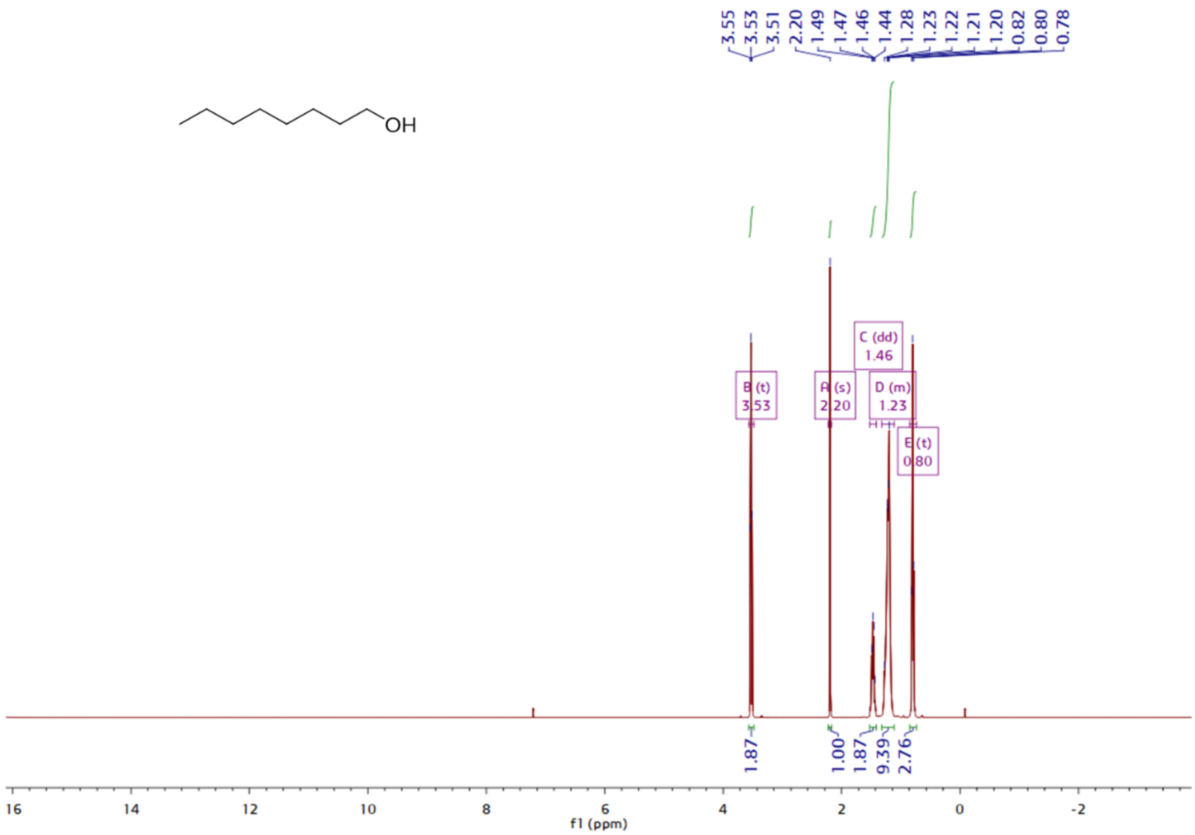


Fig.5 ^{1}H NMR

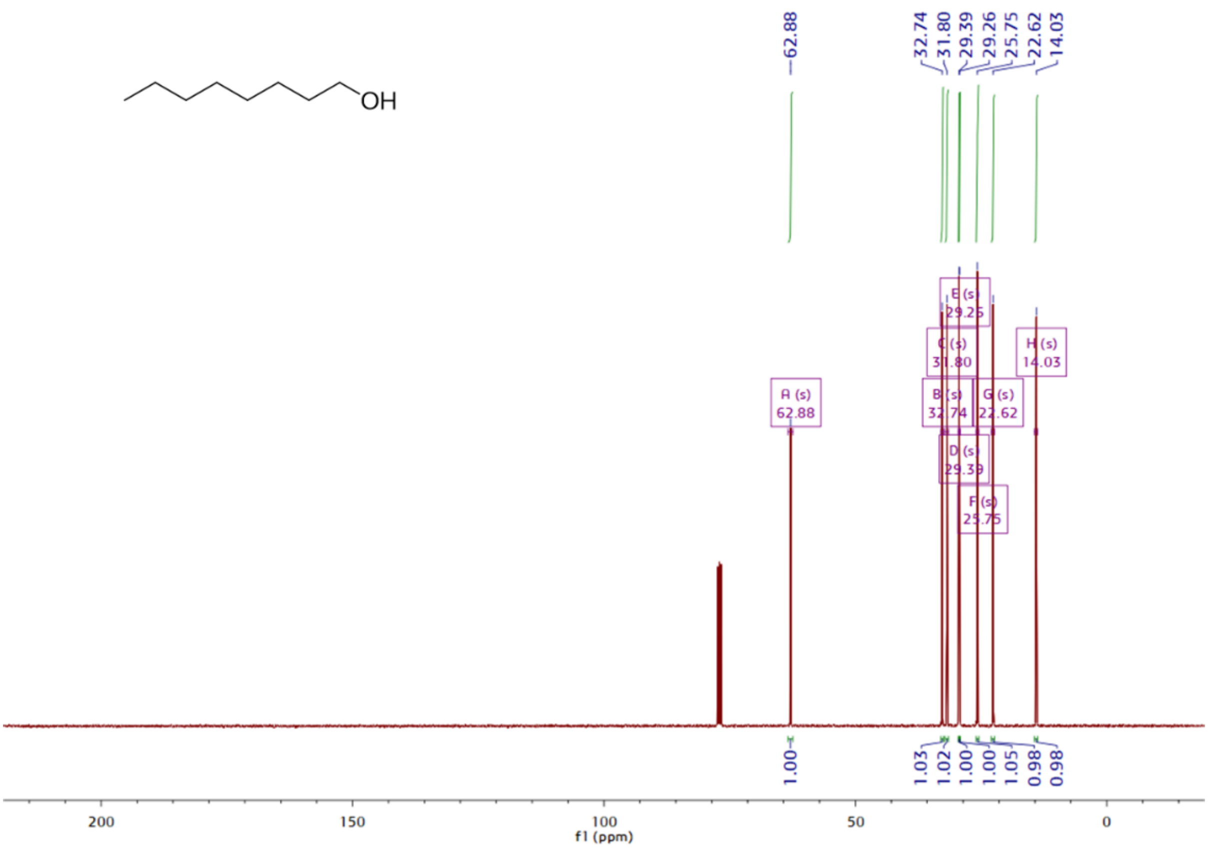


Fig.6 ^{13}C NMR

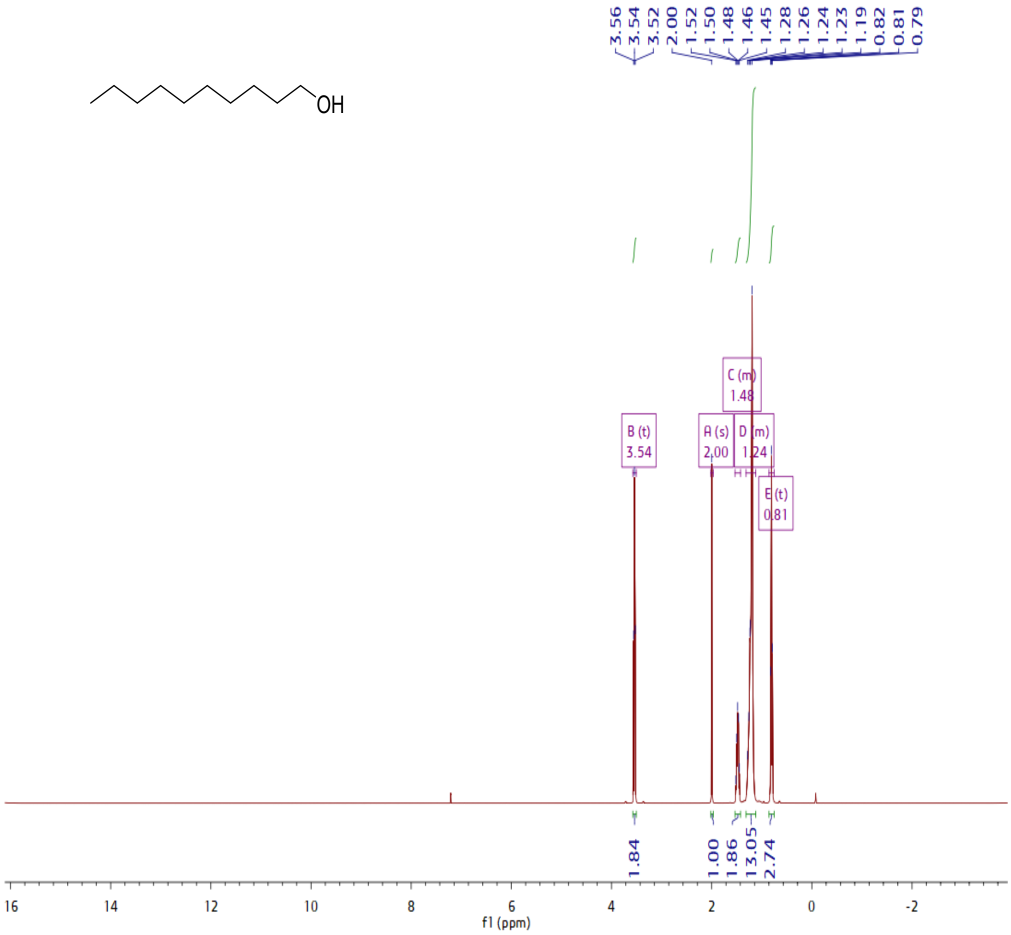


Fig.7 ^{1}H NMR

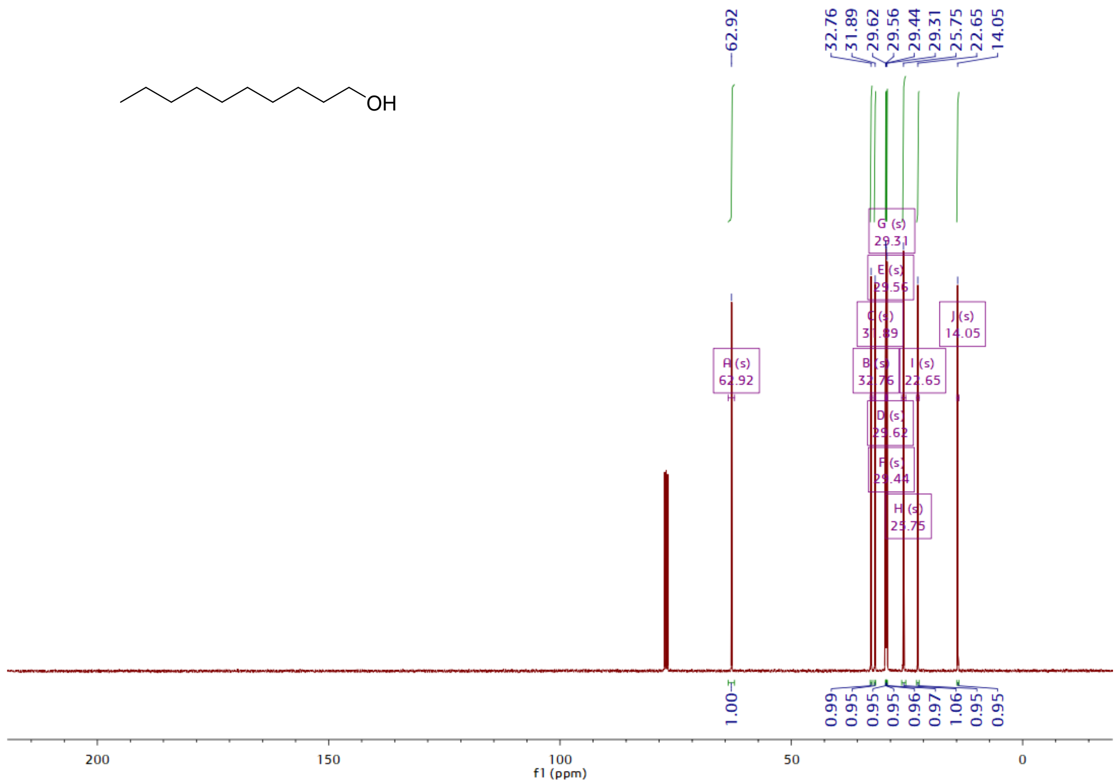


Fig.8 ^{13}C NMR

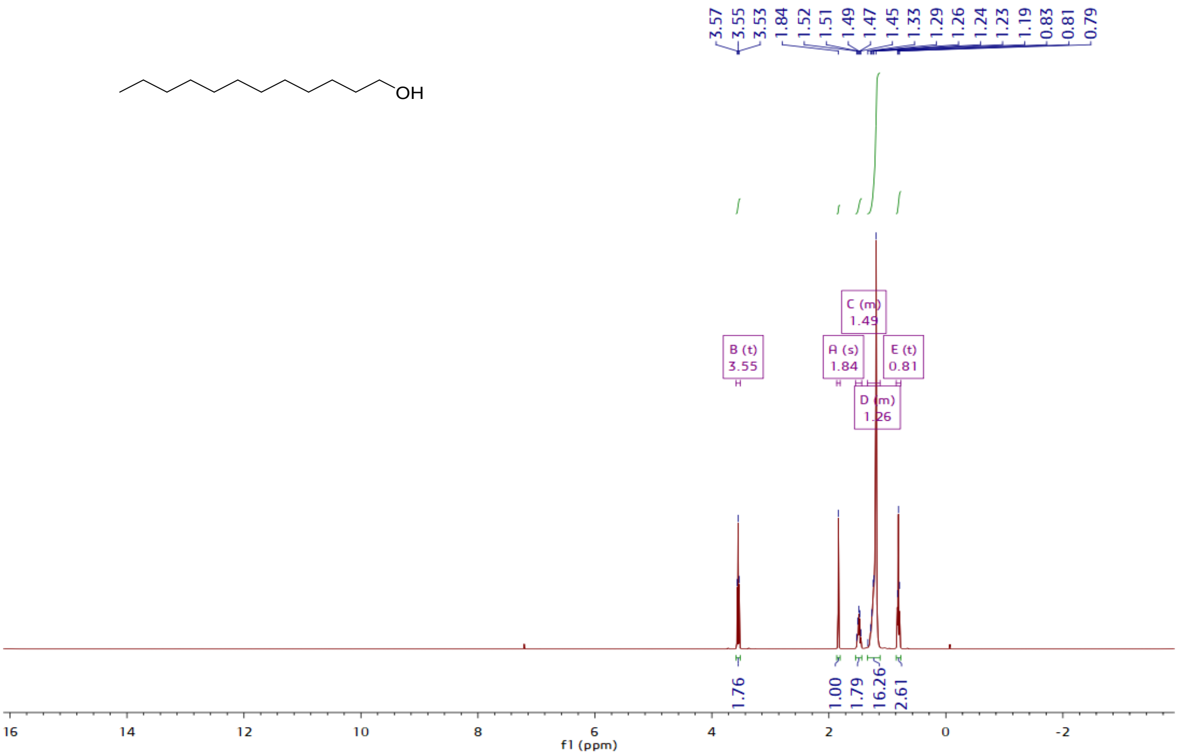


Fig.9 ^{1}H NMR

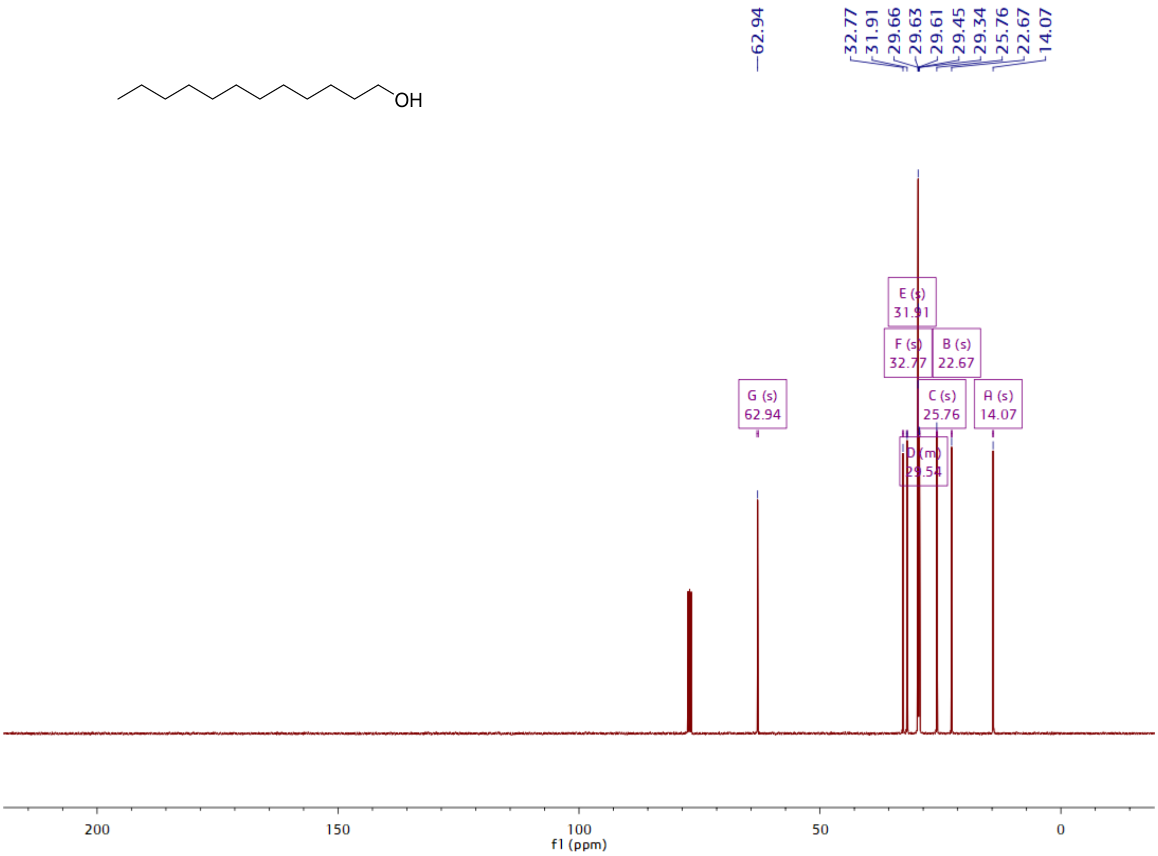


Fig.10 ^{13}C NMR

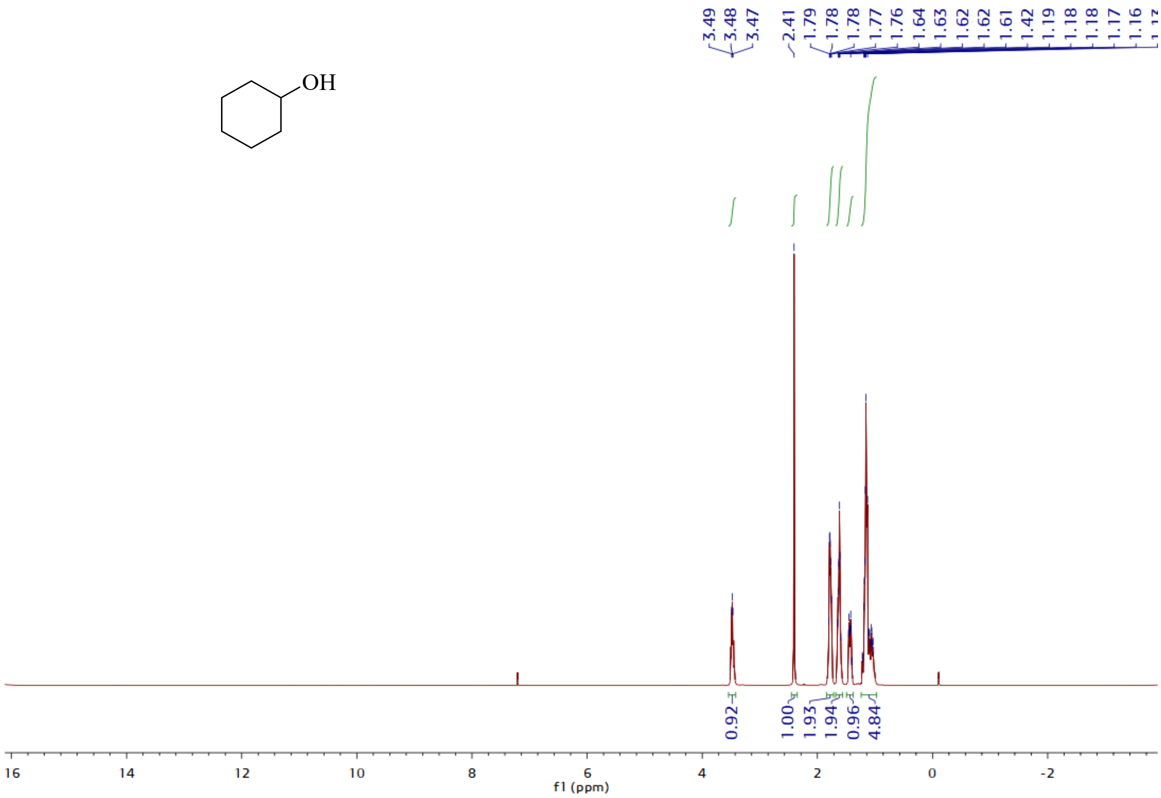


Fig.11 ^{1}H NMR

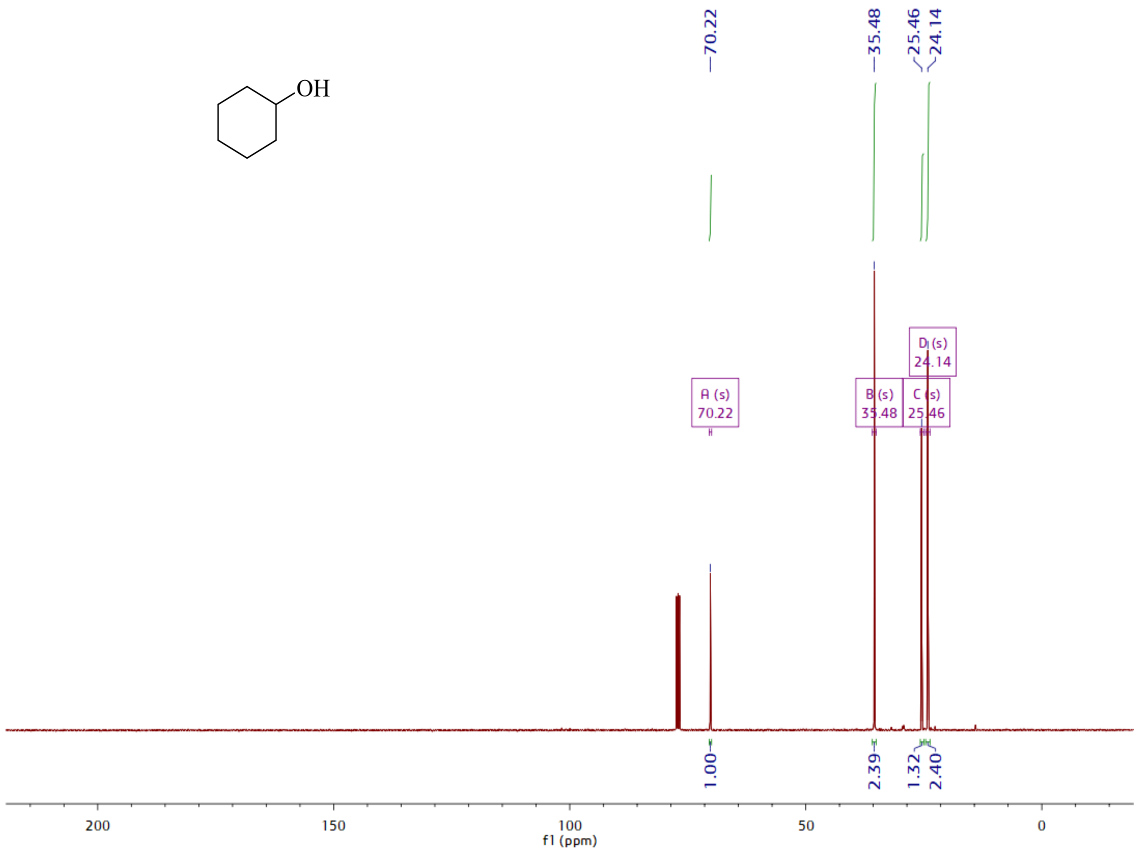


Fig.12 ^{13}C NMR

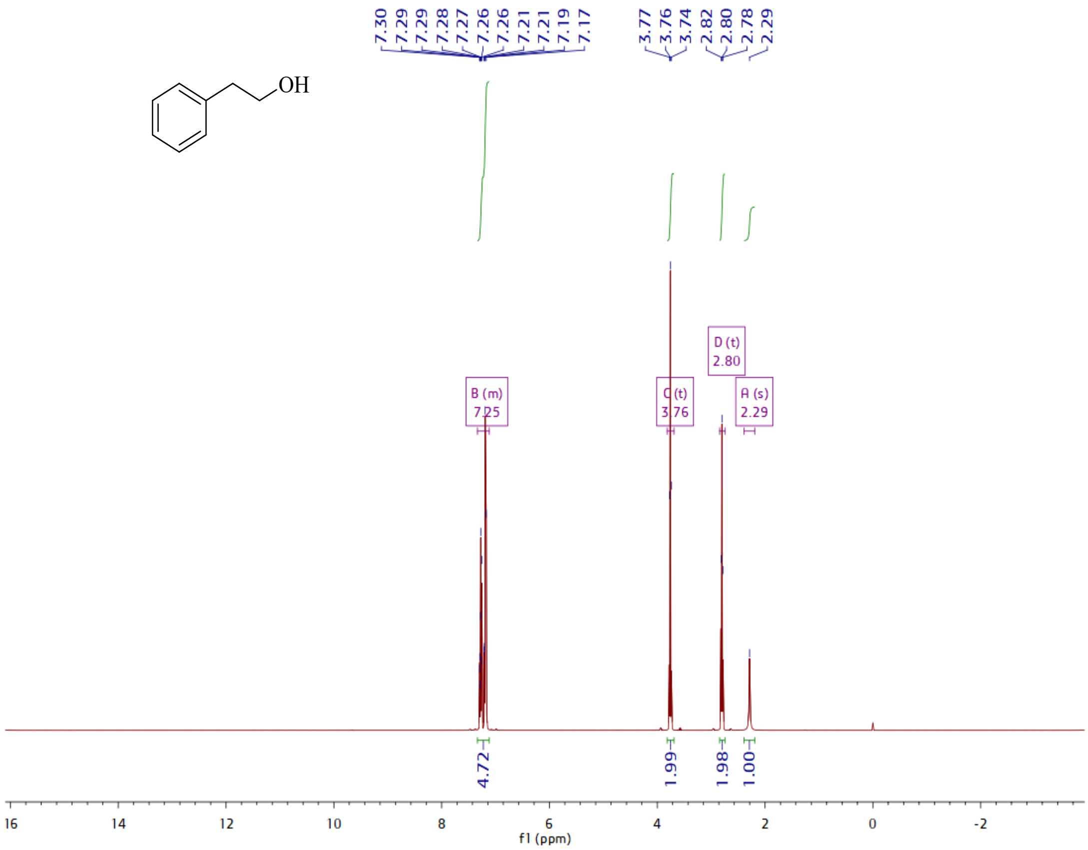


Fig.13 ^{1}H NMR

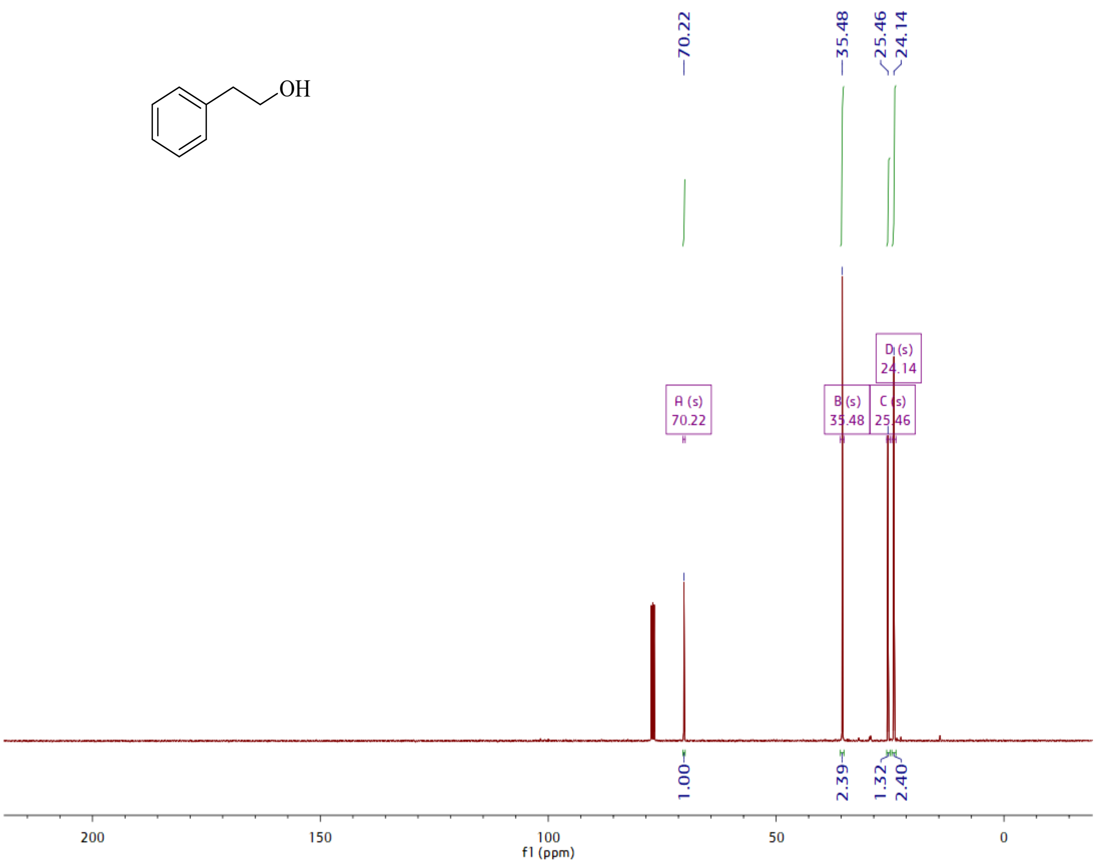


Fig.14 ^{13}C NMR

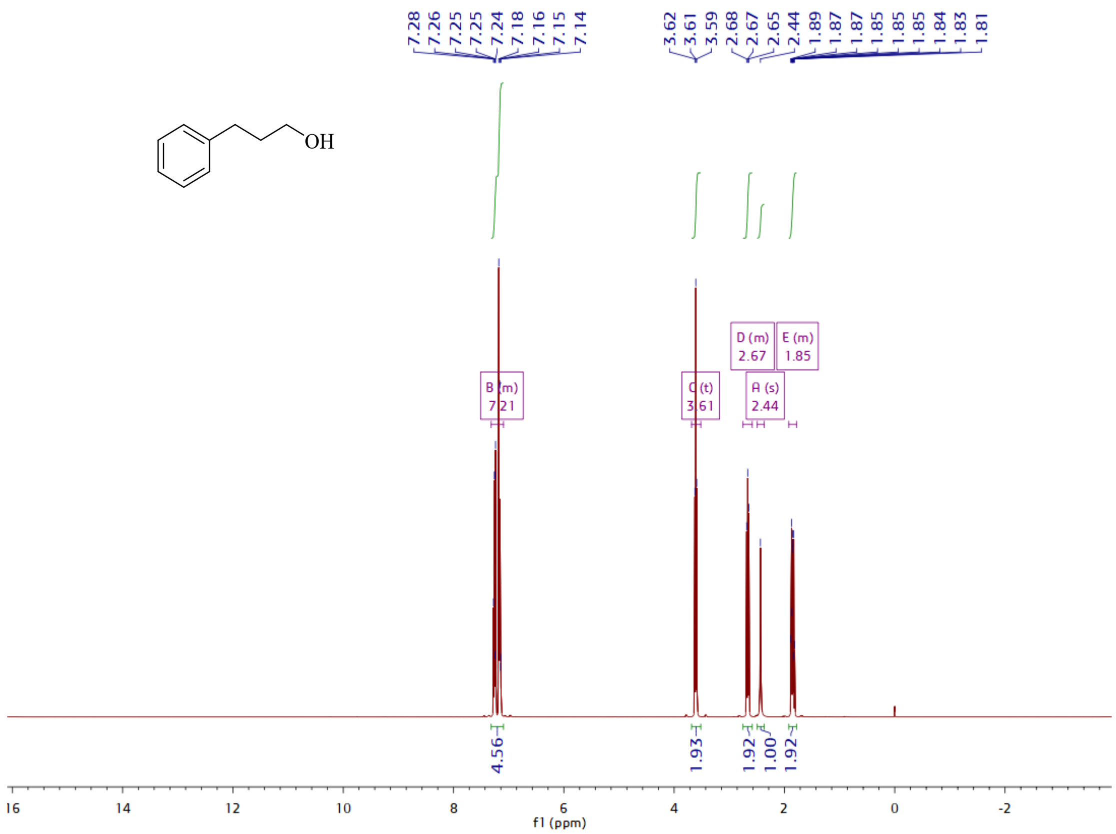


Fig.15 ^{1}H NMR

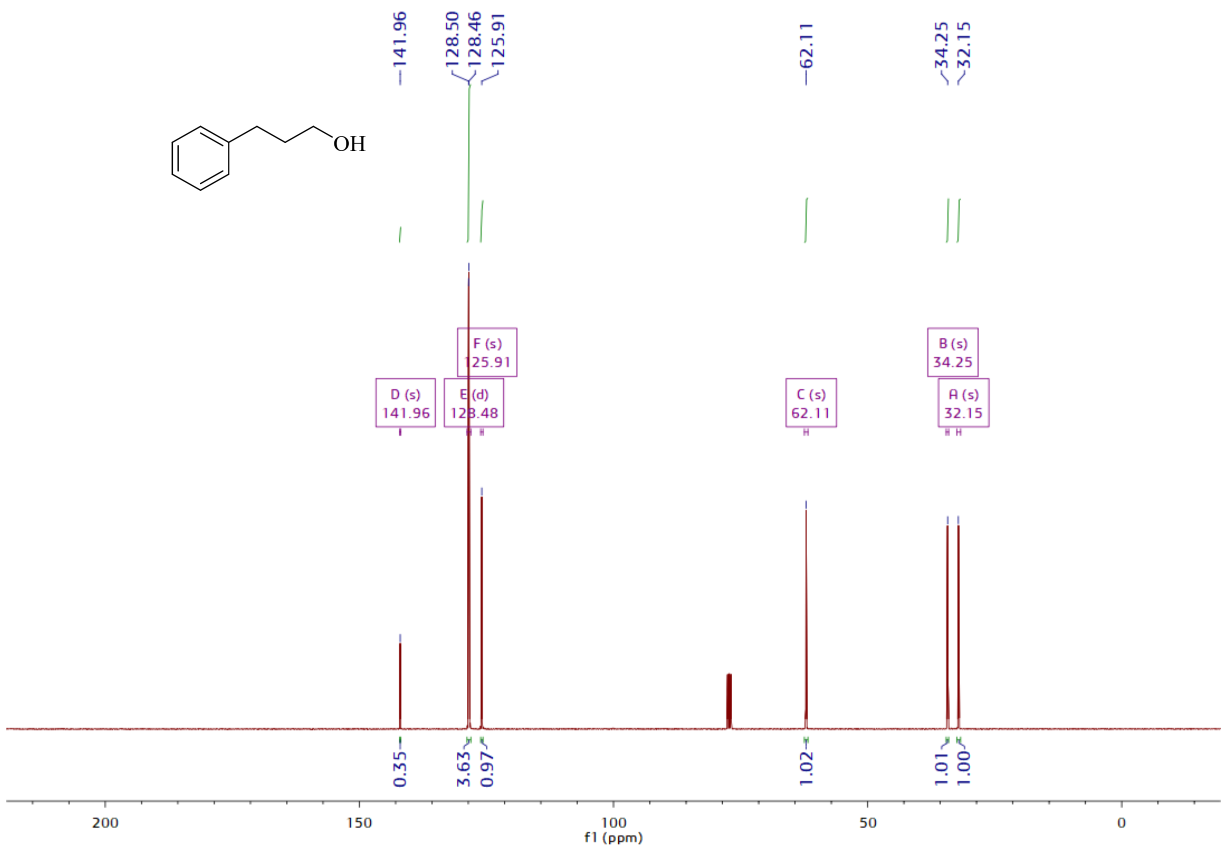


Fig.16 ^{13}C NMR

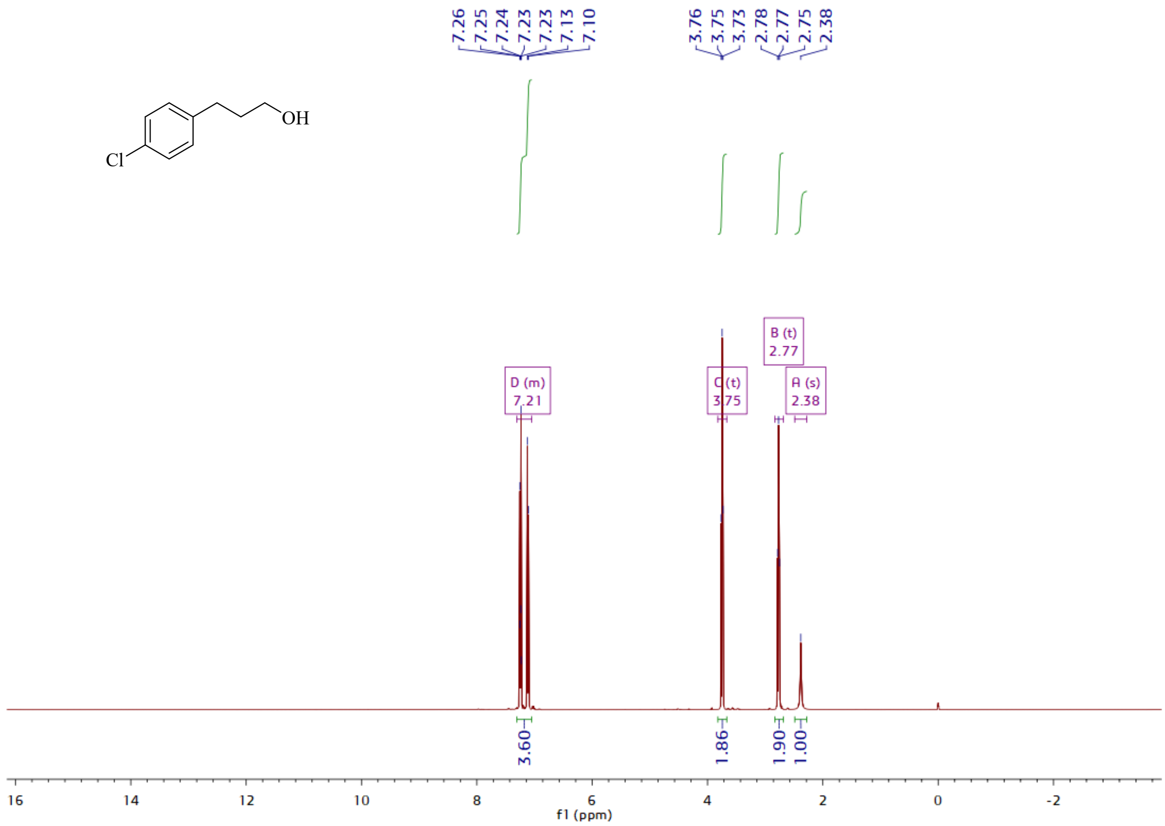


Fig.17 ^{1}H NMR

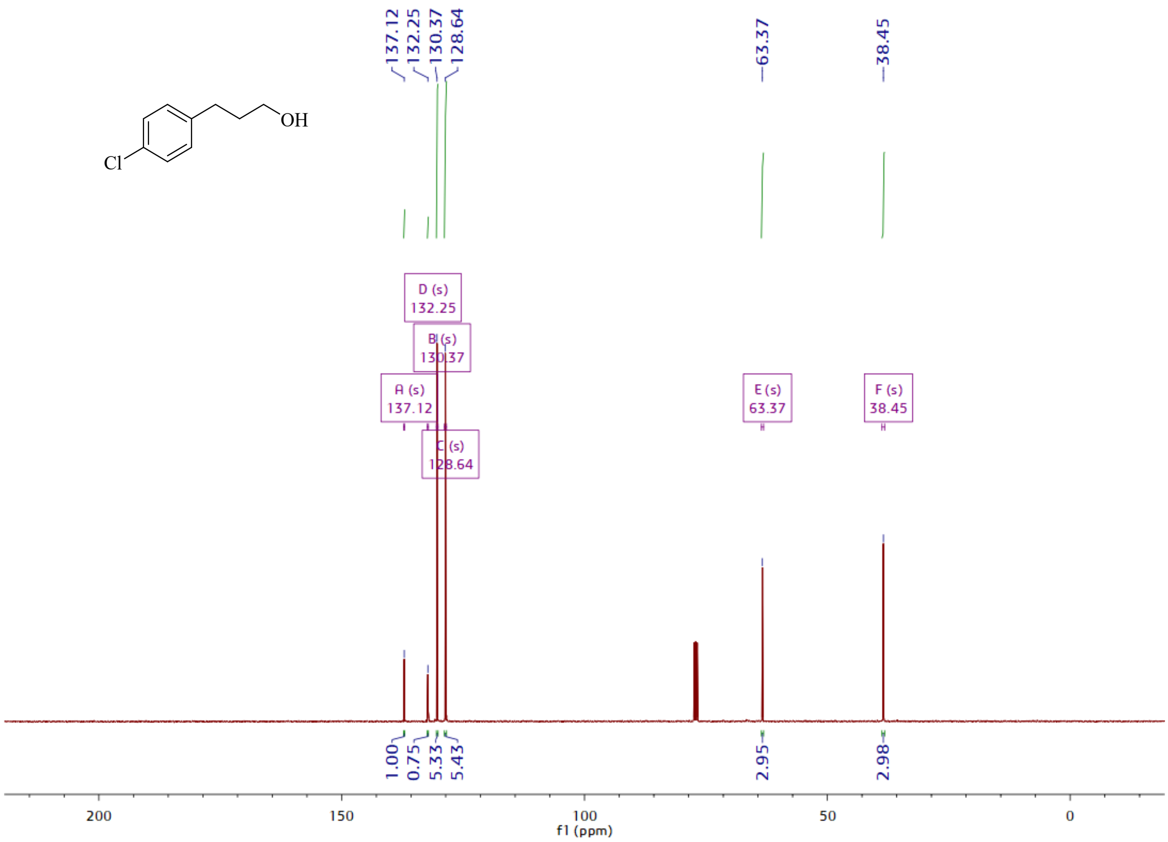


Fig.18 ^{13}C NMR

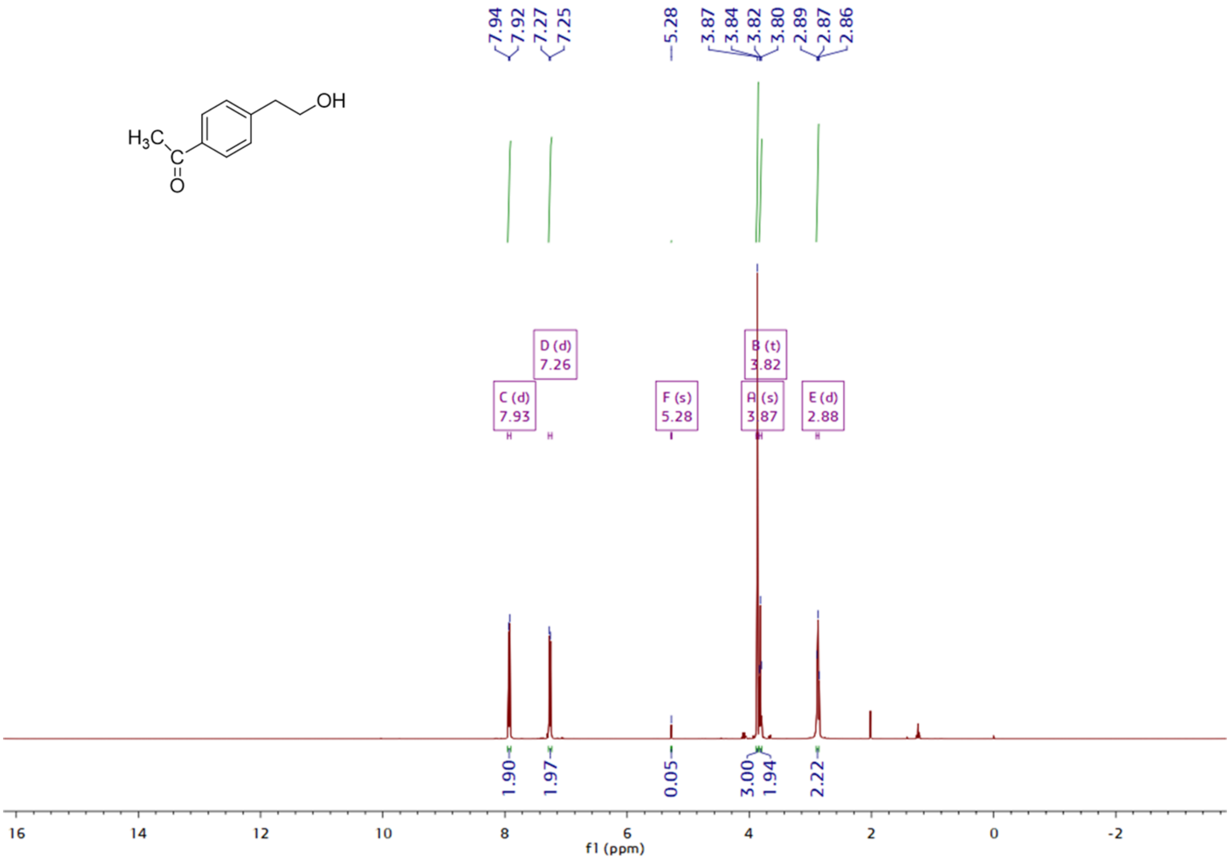


Fig.19 ^{1}H NMR

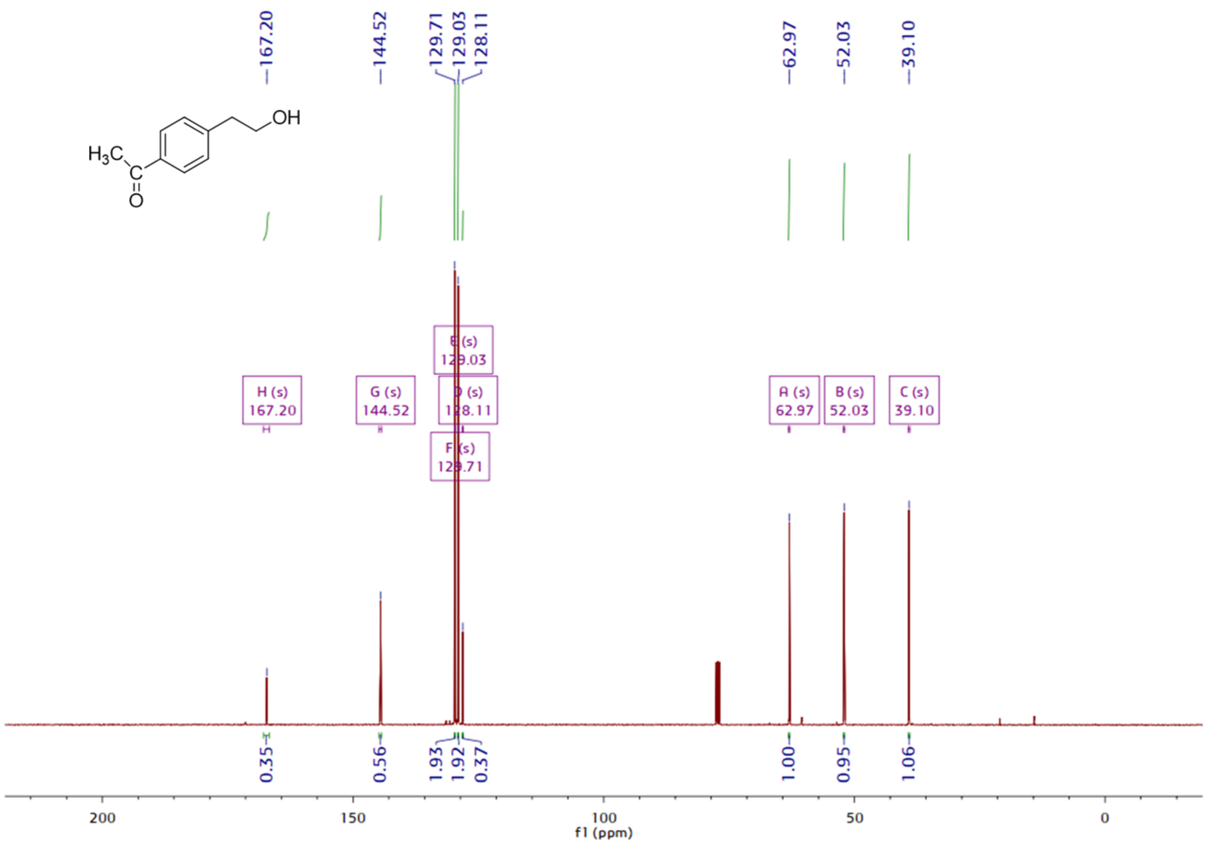


Fig.19 ^{13}C NMR

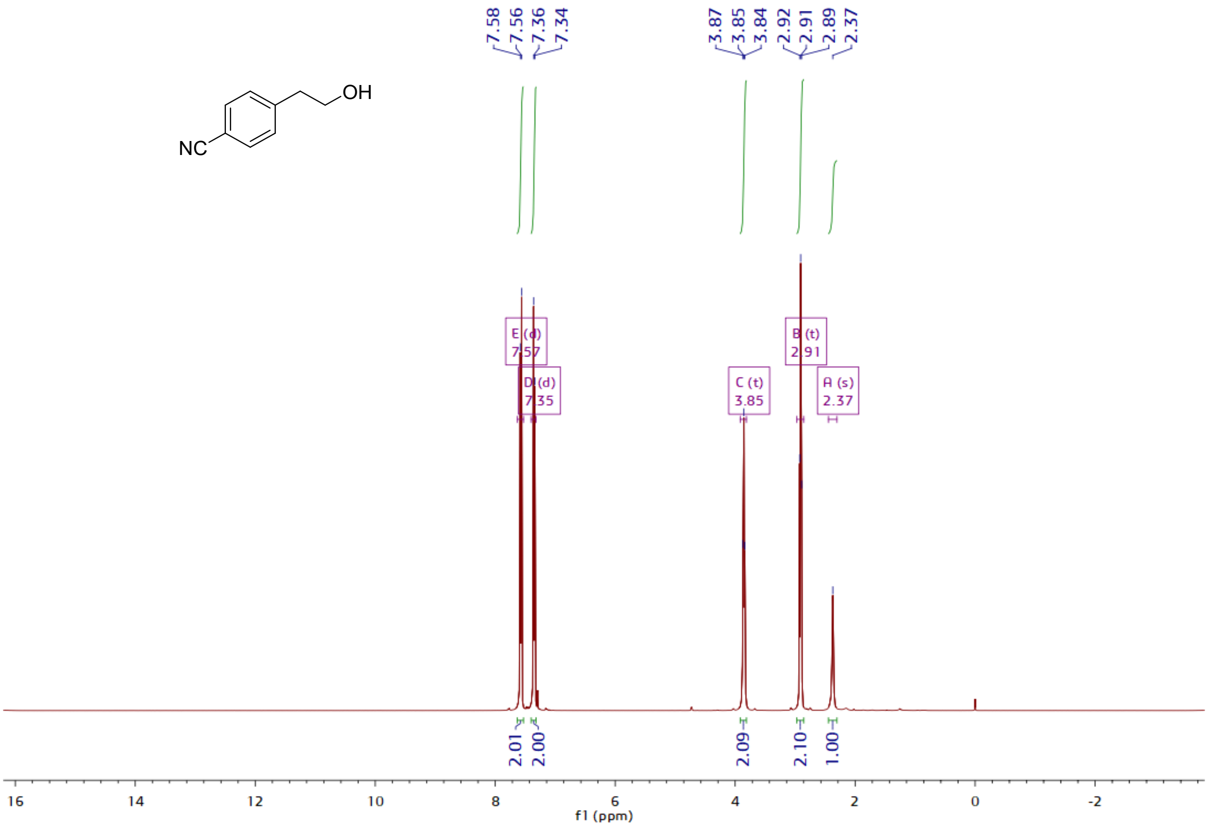


Fig.20 ^{1}H NMR

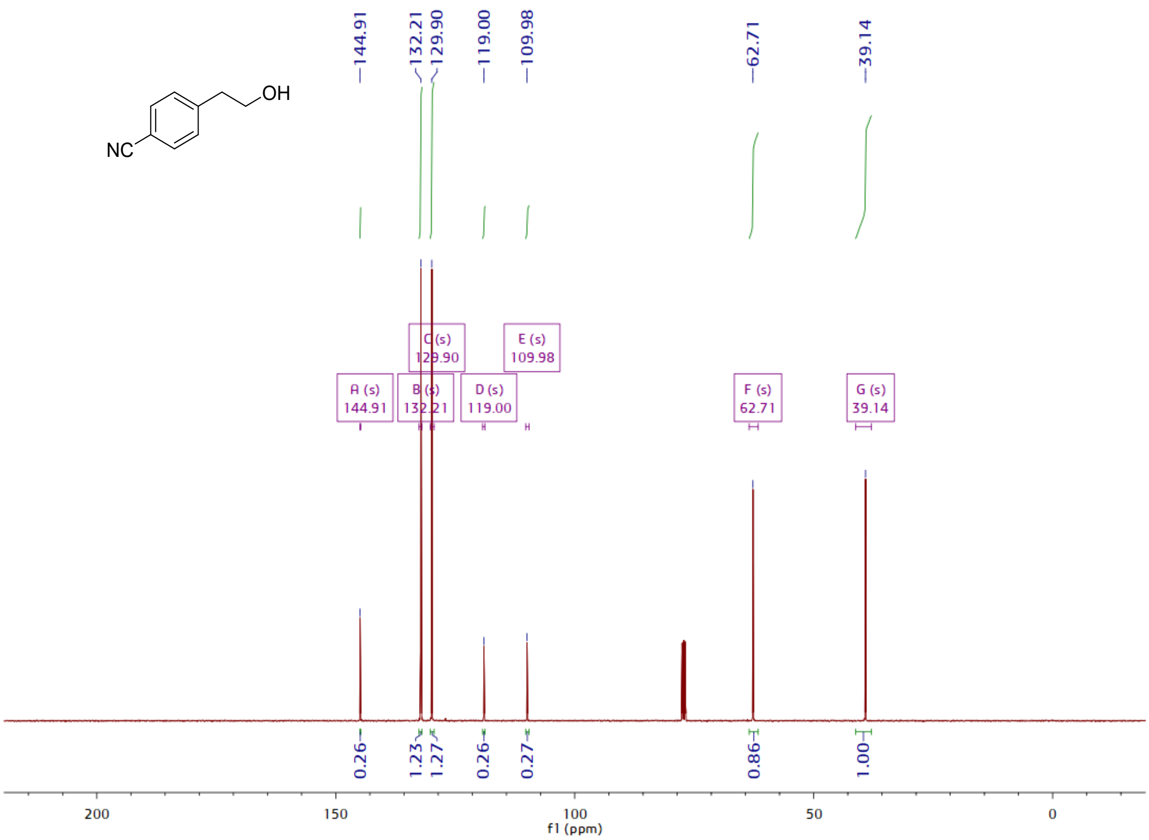


Fig.20 ^{13}C NMR