Supporting information

Facile hydrogenation of *N*-heteroarenes by magnetic nanoparticles supported sub-nanometric Rh catalysts in aqueous medium

Table 1. Structure and microstructural parameters obtained by Rietveld refinements.

Material	Phase (%)	Crystallite size (nm)	Microstrain (%)	Space group	Lattice parameter (a=b=c) (Å)	GoF
Fe_3O_4	100	8.24	0.68	*Fd-3m* (227)	8.349	1.13
Rh@Fe_3O_4	100	8.40	0.54	*Fd-3m* (227)	8.362	1.08

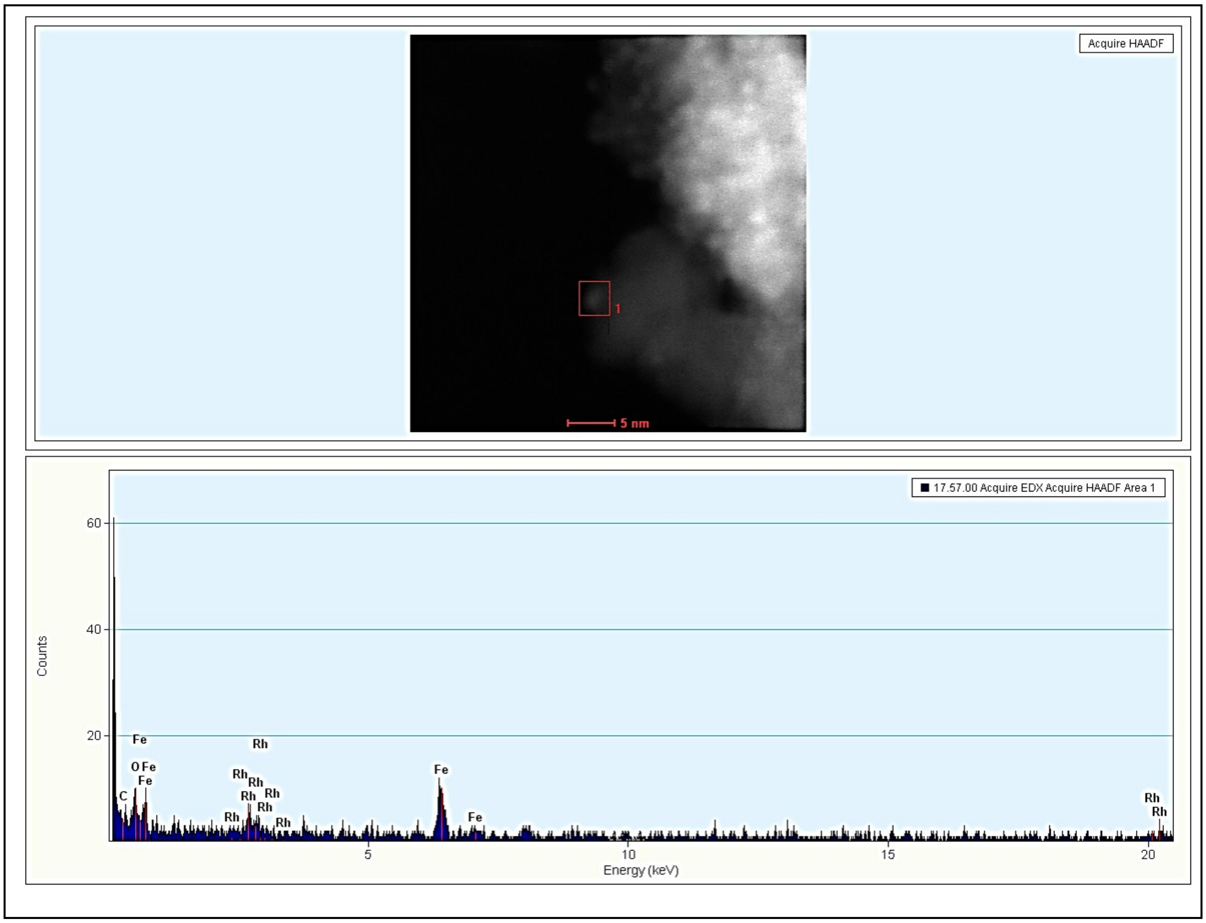


Figure S1. Identification of Rh by STEM

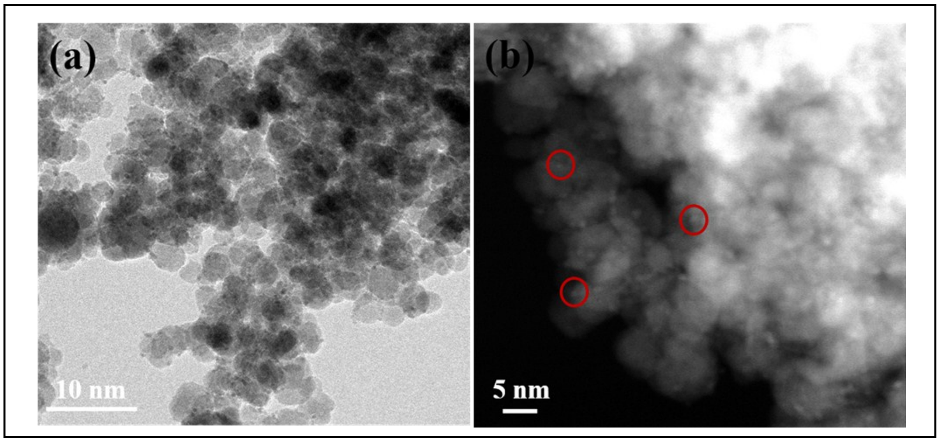


Figure S2. (a) TEM image and b) STEM image of the Rh@Fe_3O_4 after 16th use of catalyst. The red circles in (b) represents the Rh nanoparticles in it.

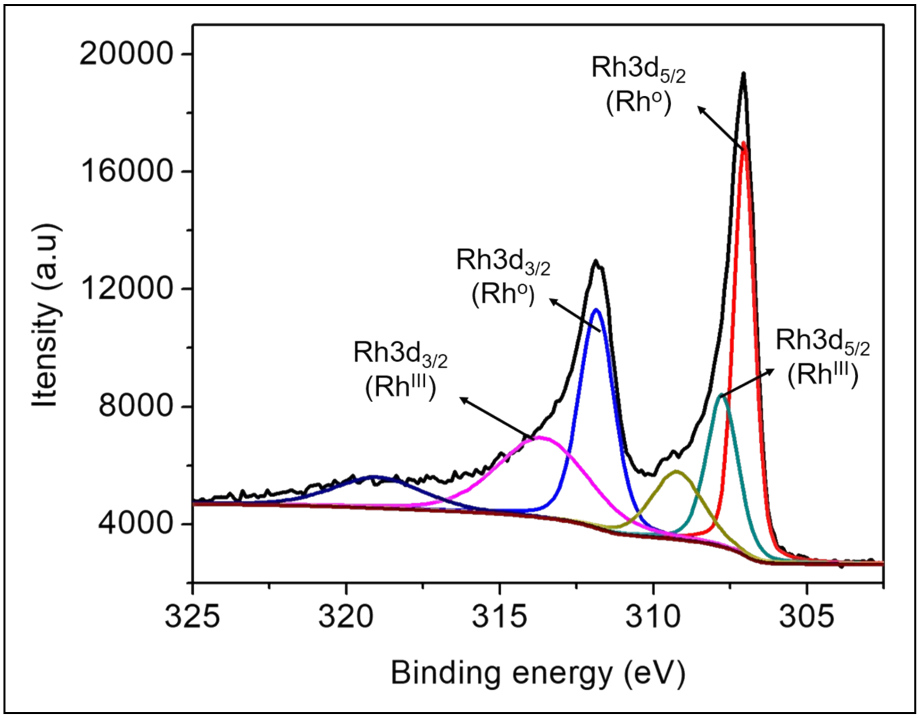


Figure S3. XPS spectrum of Rh@Fe_3O_4

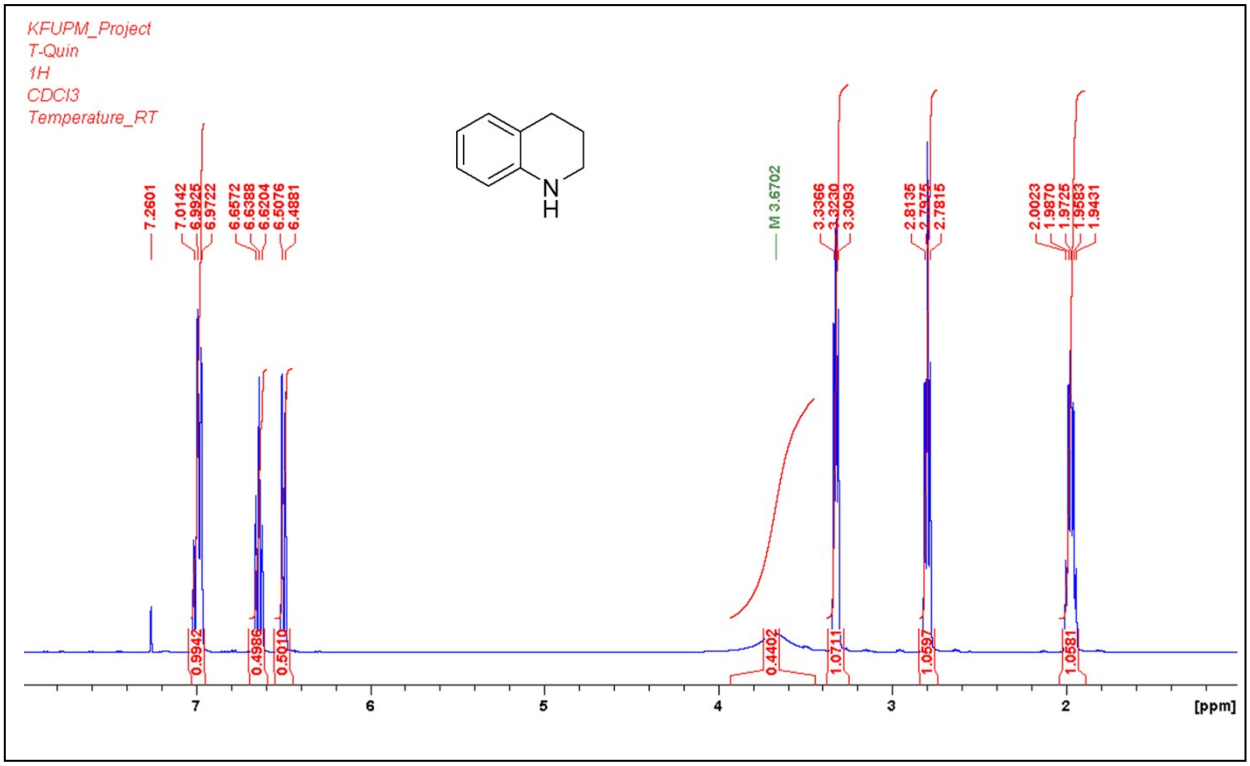


Figure S4. ^{1}H NMR of Py-THQ obtained from the Quinoline hydrogenation in water at 80 ^{o}C using tetrahydroxydiboron (THDB)

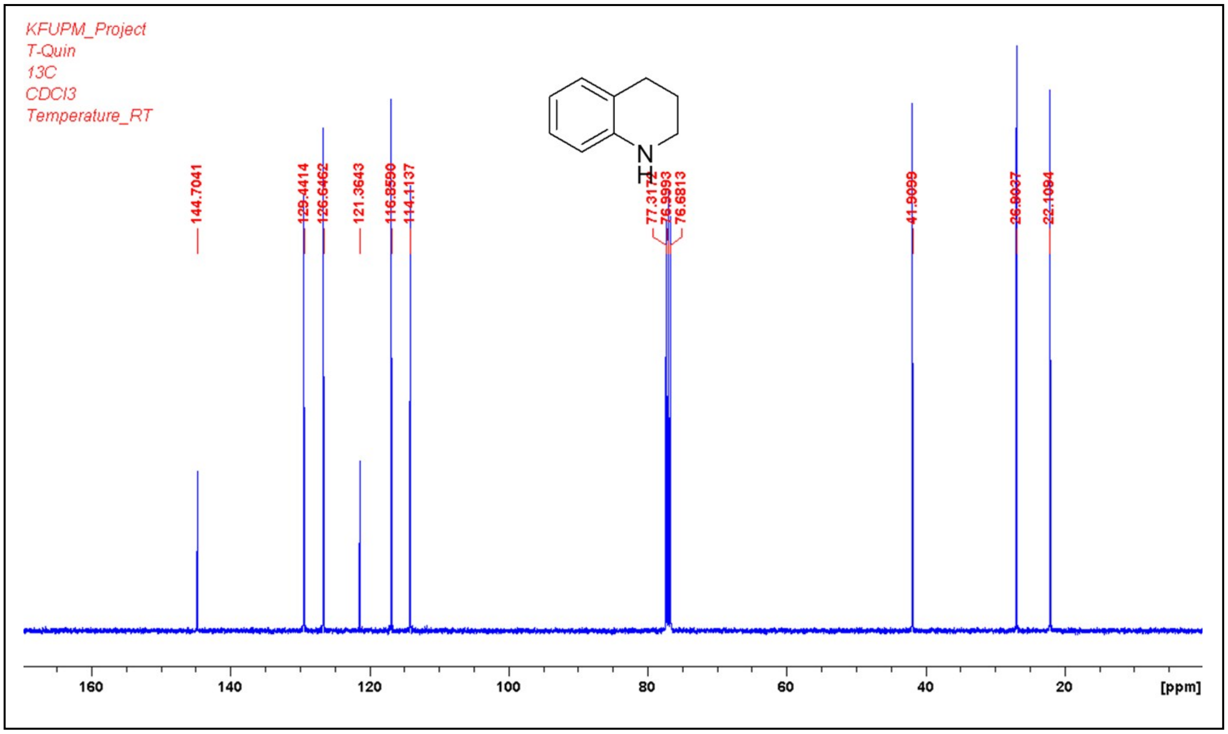


Figure S5. ^{13}C NMR of Py-THQ obtained from the Quinoline hydrogenation in water at 80 ^oC using tetrahydroxydiboron (THDB)

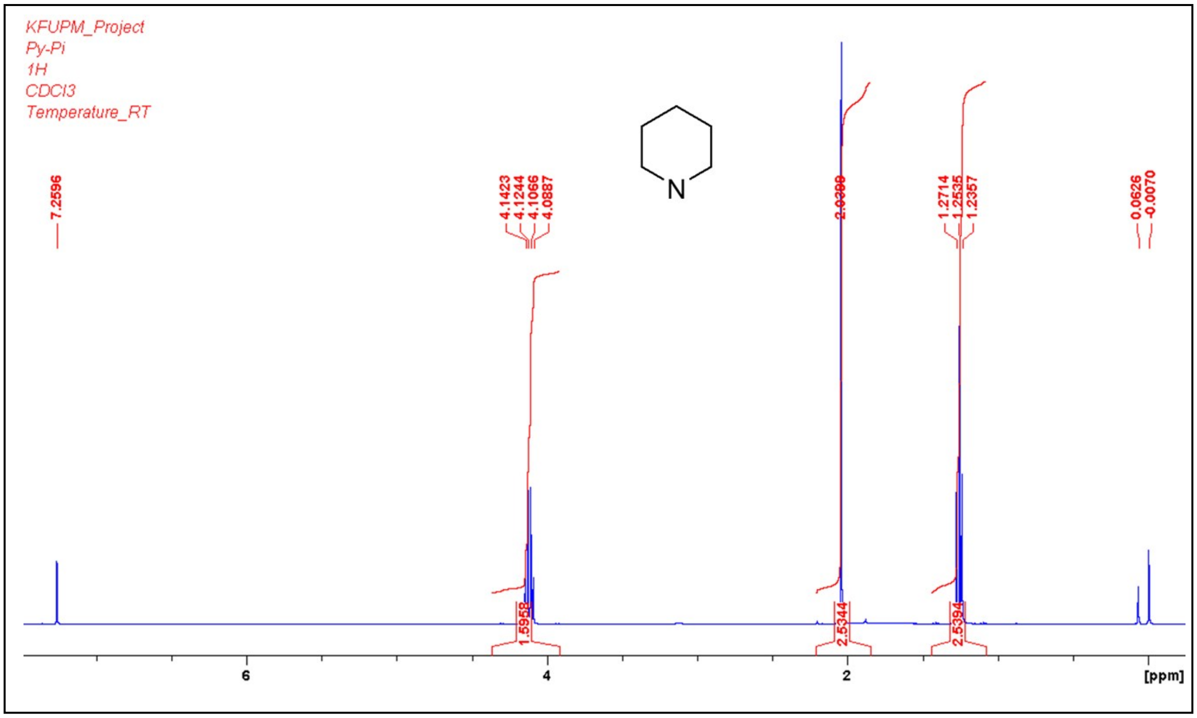


Figure S6. [1]H NMR of Piperidine obtained from the pyridine hydrogenation under molecular hydrogen pressure.

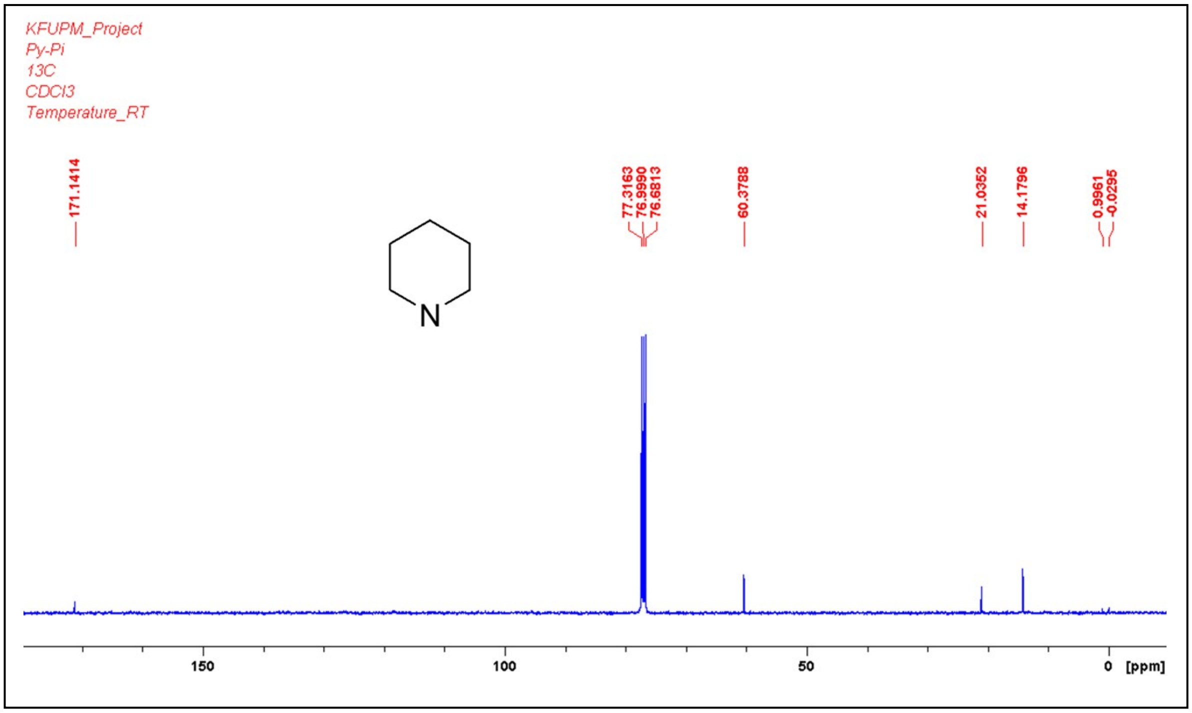


Figure S7. ^{13}C NMR of Piperidine obtained from the pyridine hydrogenation under molecular hydrogen pressure.

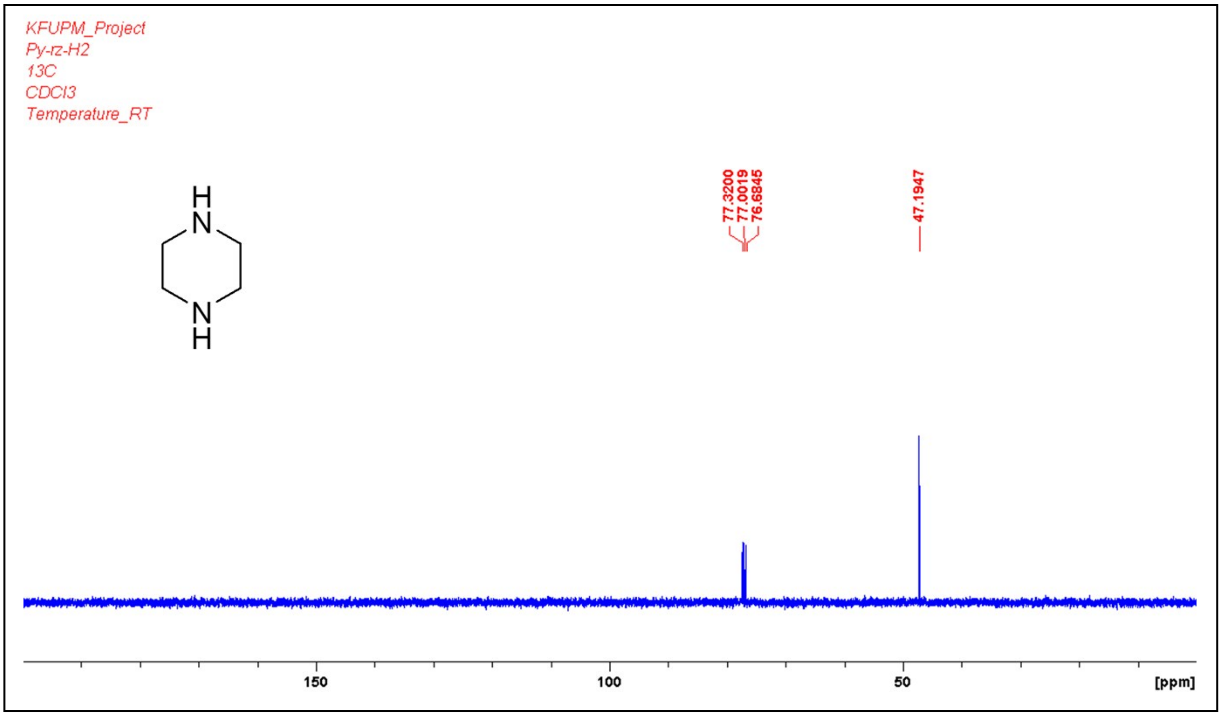


Figure S8. ^{13}C NMR of piperazine obtained from the pyrazine hydrogenation under molecular hydrogen pressure.

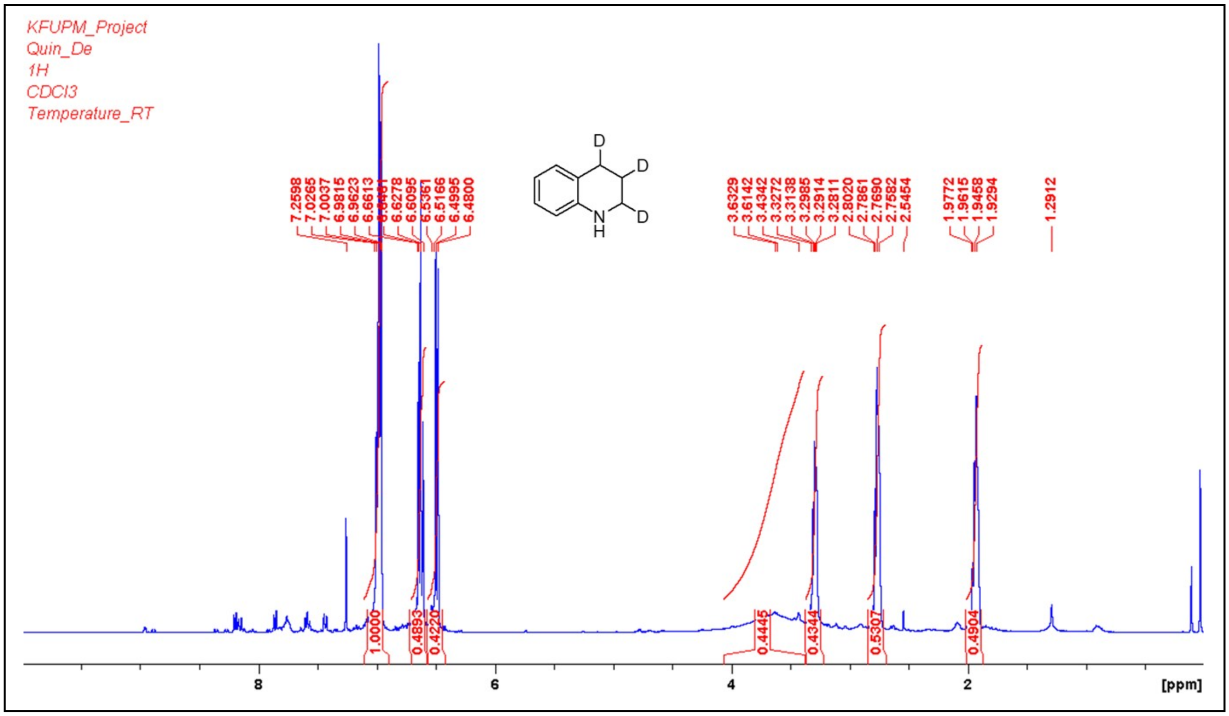


Figure S9. ^{1}H NMR of Py-THQ obtained from the Quinoline hydrogenation in D_2O at 80 ^{o}C using tetrahydroxydiboron (THDB).

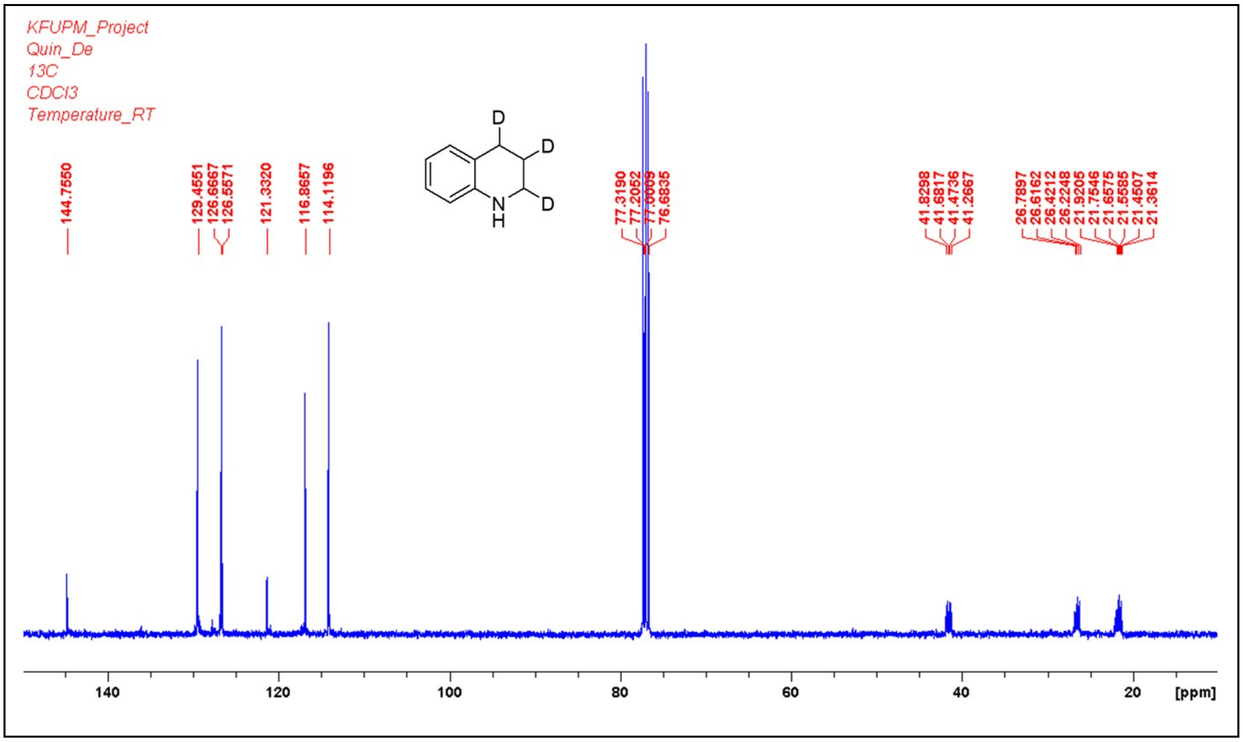
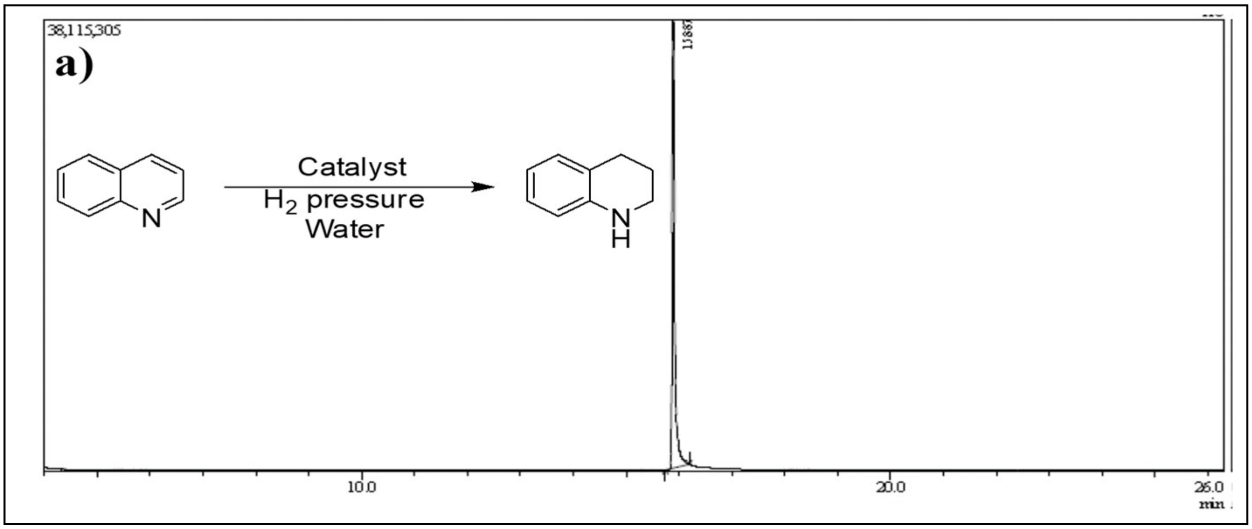


Figure S10. ^{13}C NMR of Py-THQ obtained from the Quinoline hydrogenation in D_2O at 80 ^{o}C using tetrahydroxydiboron (THDB).



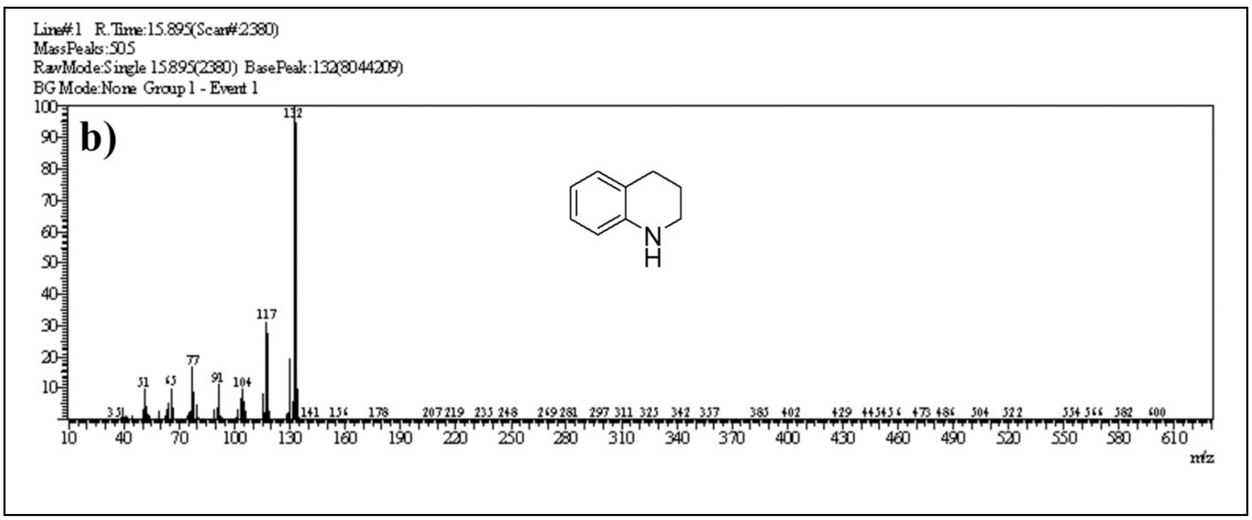


Figure S11. GC and GCMS spectrum of Quinoline hydrogenation under molecular hydrogen pressure in water at 50 ^oC.

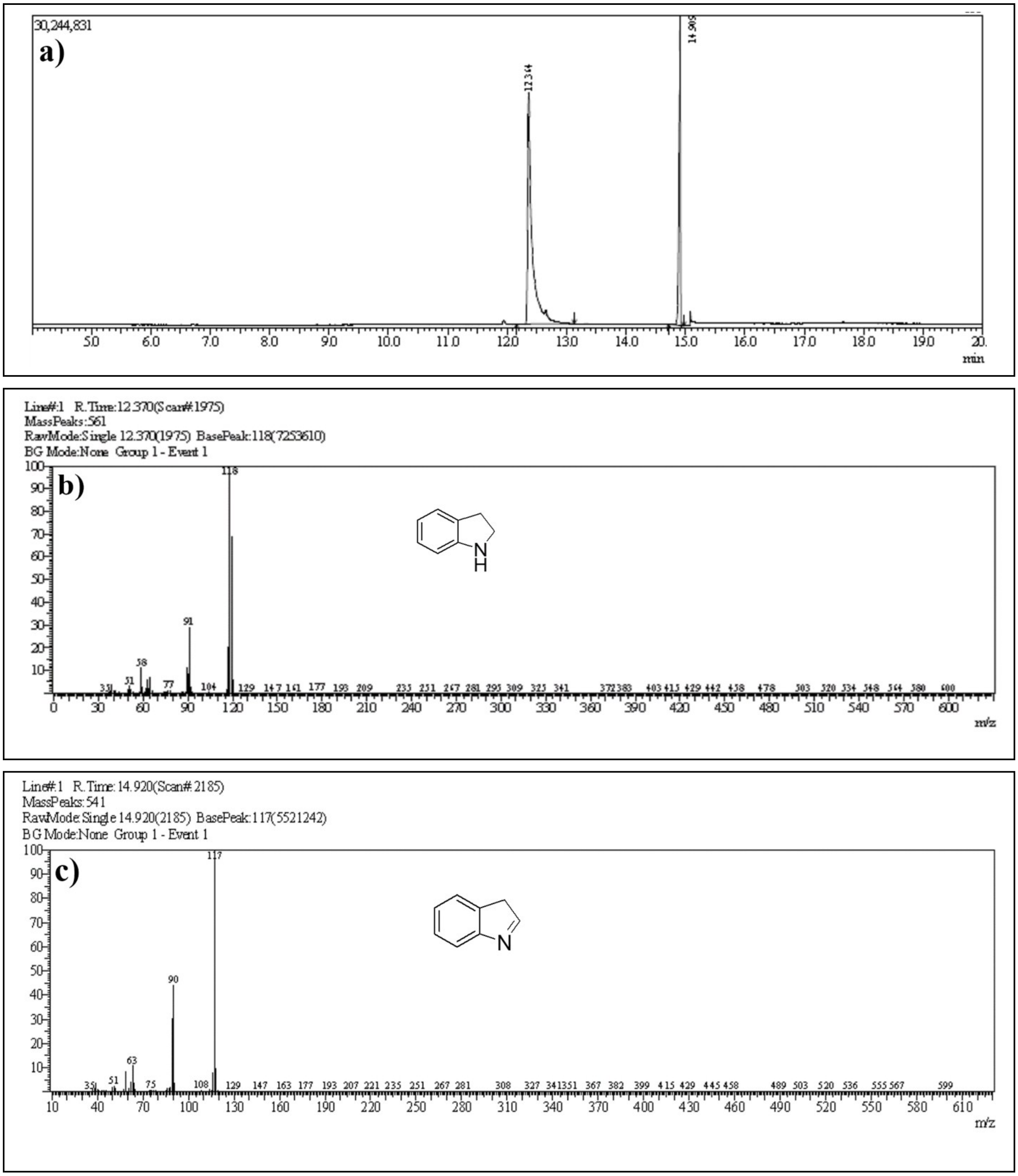
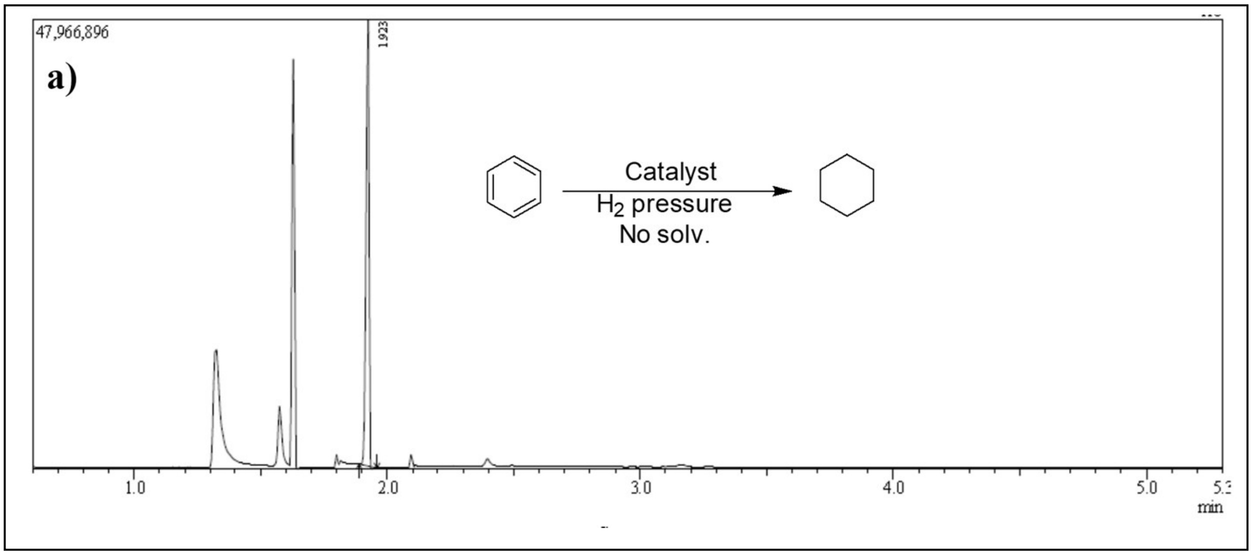


Figure S12. GC and GCMS spectrum of indole hydrogenation under molecular hydrogen pressure in THF at 140 ^{o}C under 40 bar H_2 pressure.



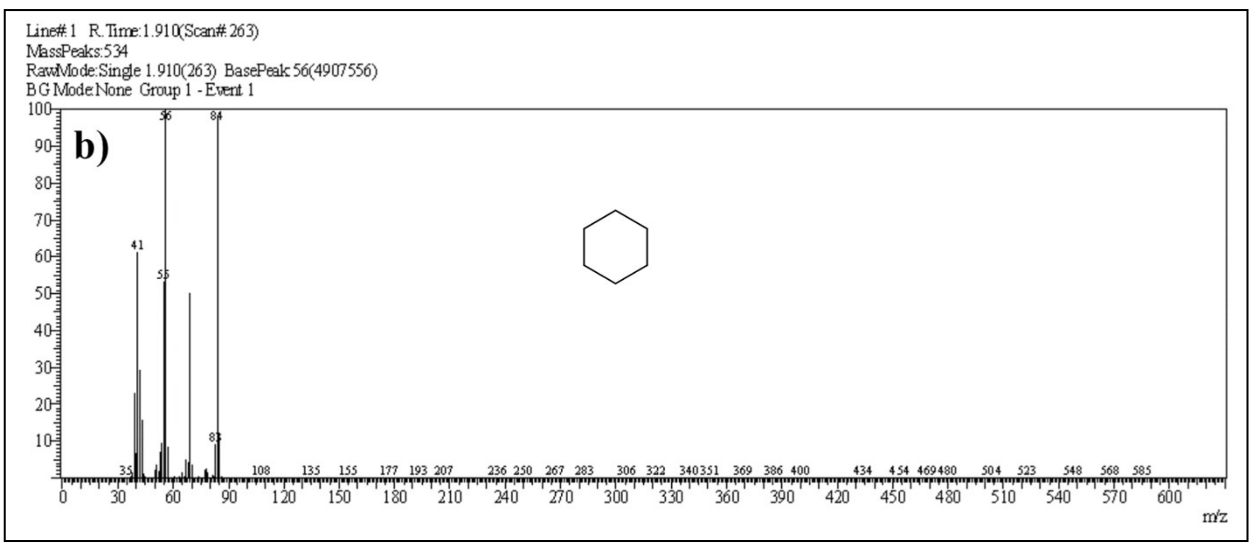


Figure S13. GC and GCMS spectrum of benzene hydrogenation under molecular hydrogen pressure at 100 ^{o}C without solvent.

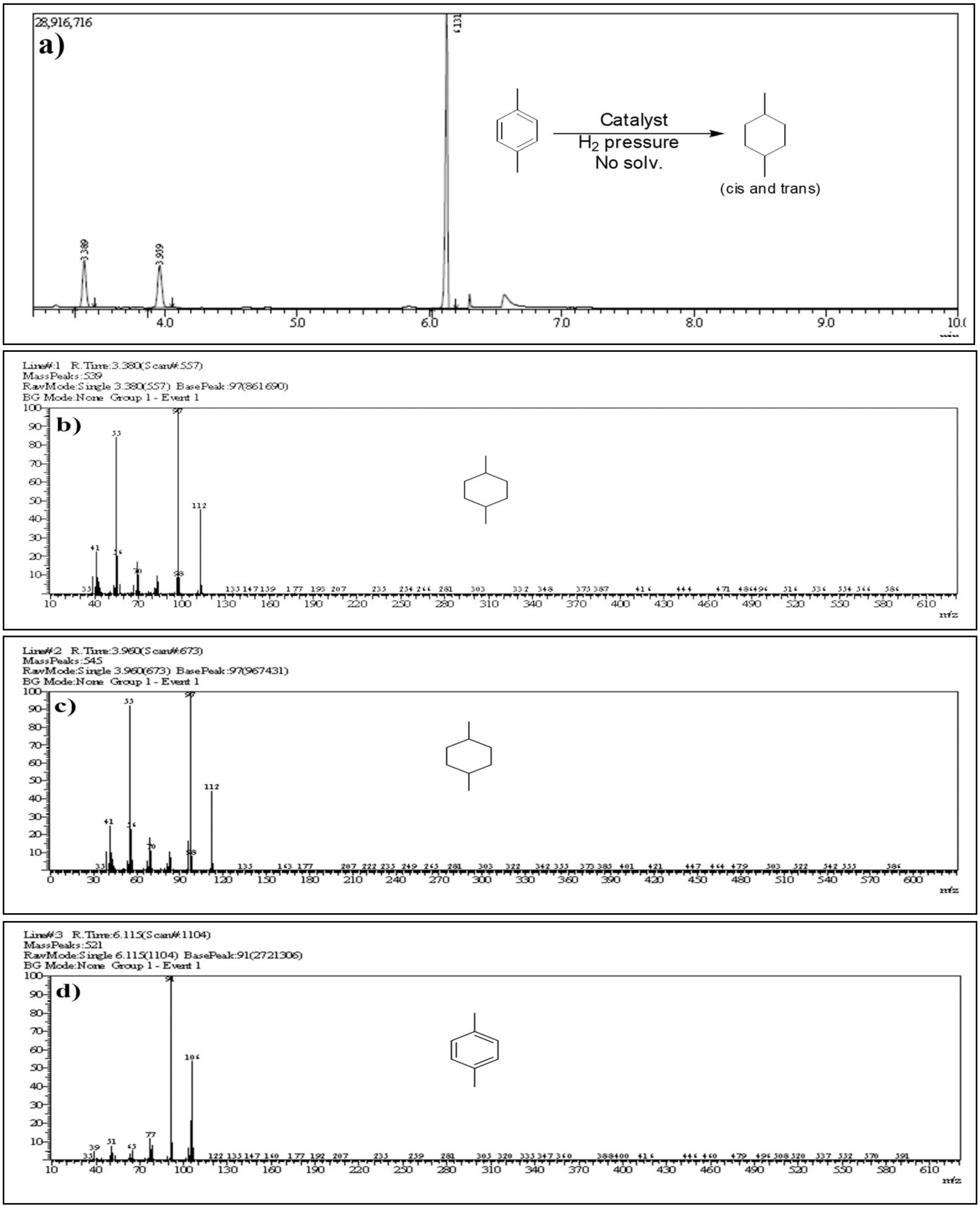

28,916,716
a)
Catalyst
H_2 pressure
No solv.
(cis and trans)
Line#:1 R.Time:3.380(Scan#:557)
MassPeaks:539
RawMode:Single 3.380(557) BasePeak:97(861690)
BG Mode:None Group 1 - Event 1
b)
Line#:2 R.Time:3.960(Scan#:673)
MassPeaks:545
RawMode:Single 3.960(673) BasePeak:97(967431)
BG Mode:None Group 1 - Event 1
c)
Line#:3 R.Time:6.115(Scan#:1104)
MassPeaks:521
RawMode:Single 6.115(1104) BasePeak:91(2721306)
BG Mode:None Group 1 - Event 1
d)
m/z

Figure S14. GC and GCMS spectrum of p-xylene hydrogenation under molecular hydrogen pressure without solvent at 130 ^{o}C under 40 bar H_2 pressure.

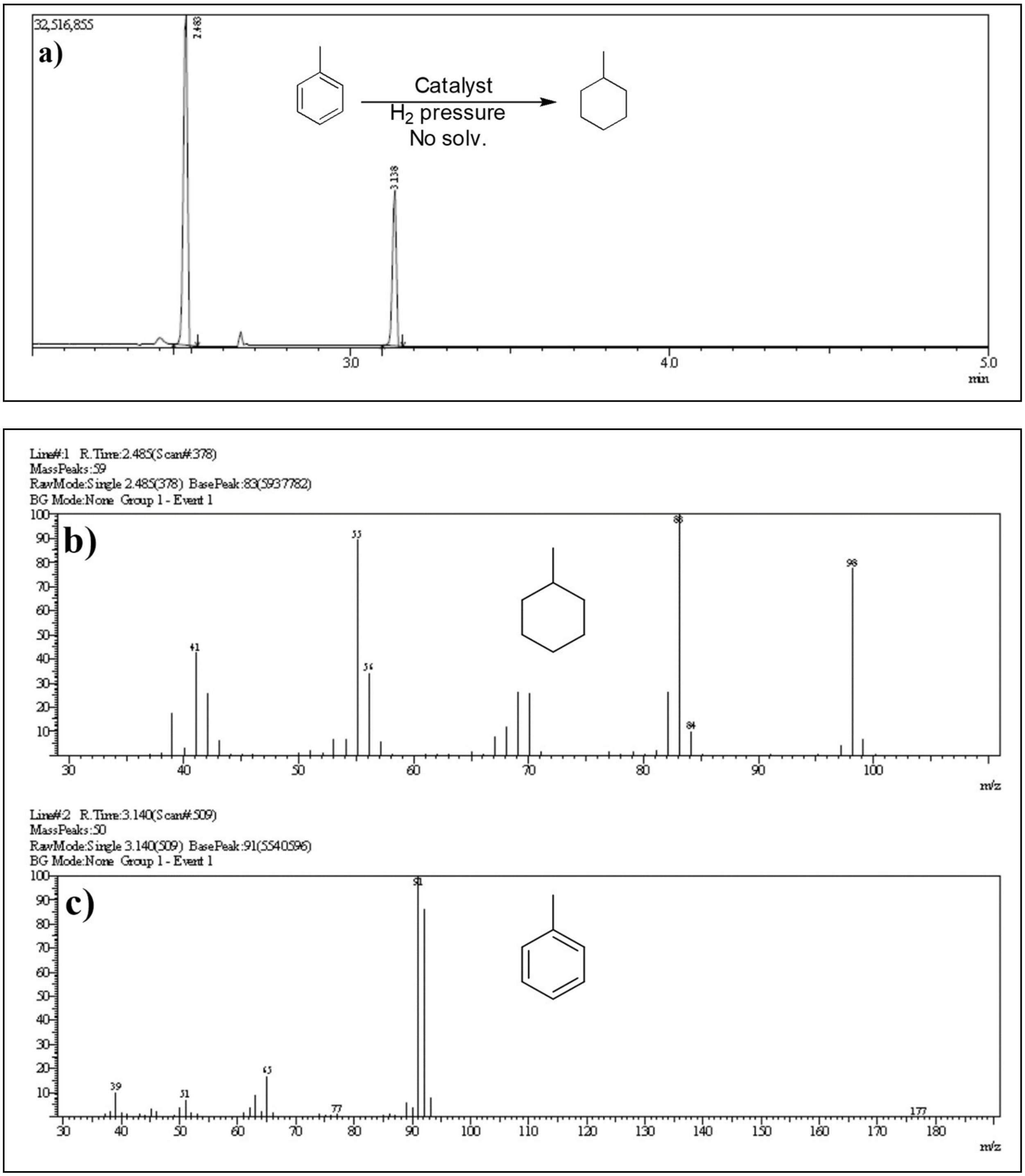


Figure S15. GC and GCMS spectrum of toluene hydrogenation under molecular hydrogen pressure without solvent at 130 ^oC under 40 bar H_2 pressure.

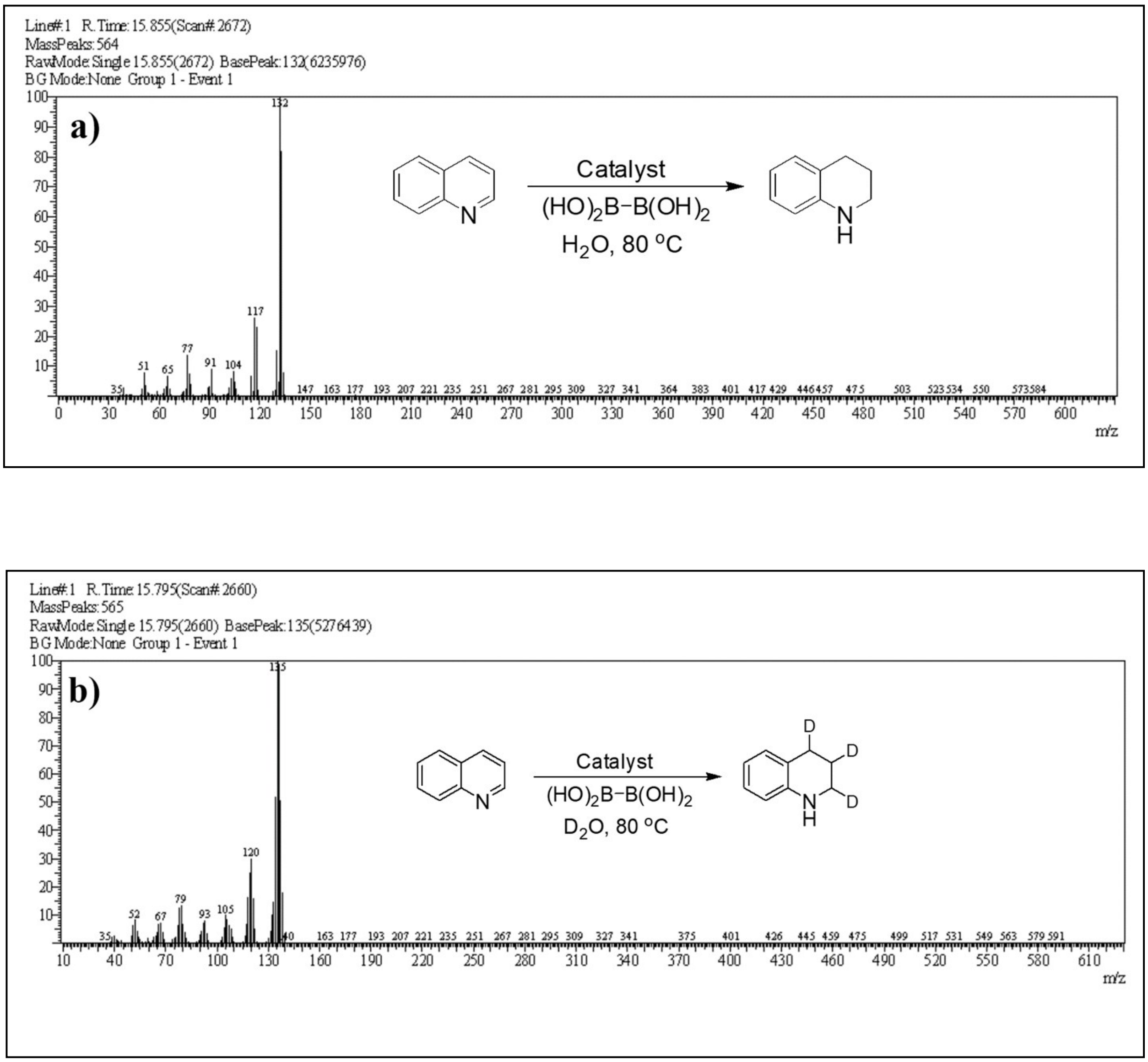


Figure S16. GCMS spectra of reduced product a) py-THQ and b) deuterated py-THQ in presence of tetrahydroxydiboron in H_2O and D_2O respectively.