Supporting Information

In situ Approach for Testing the Enantiopurity of Chiral Amines and Amino Alcohols by ^{1}H NMR

Sandeep Kumar Mishra, Sachin R. Chaudhari, and N. Suryaprakash*

NMR Research Centre, Solid State and Structural Chemistry Unit,

Indian Institute of Science, Bangalore-560012

*Corresponding Author

e-mail: nsp@nrc.iisc.ernet.in
Tel: 0091 80 22933300, 919845124802
Fax: 0091 8023601550

Table of contents pages

NMR spectra

Figure S1: ^{1}H-NMR spectrum of (*R/S*)-4-fluoro-α-methylbenzylamine.

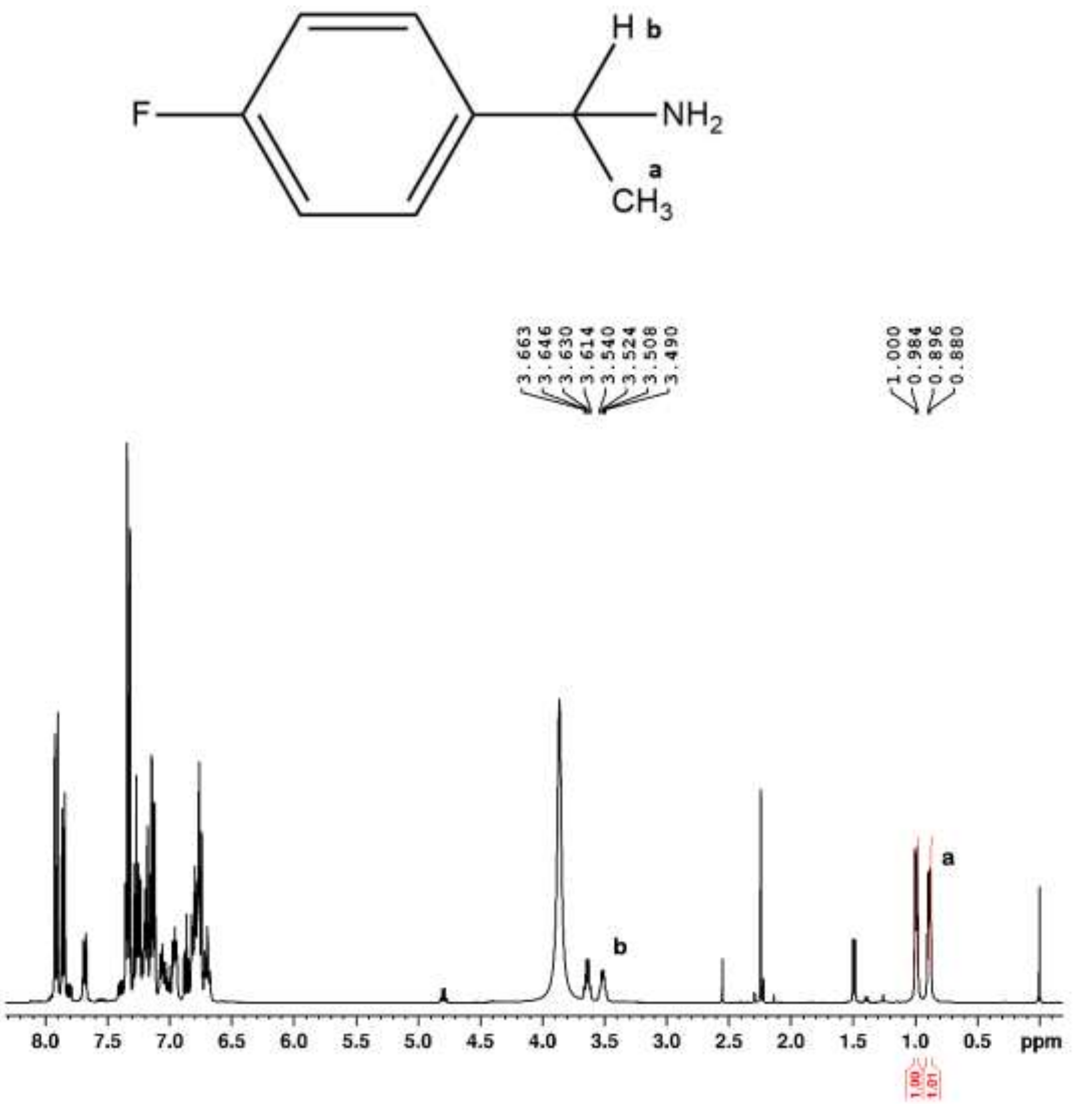


Figure S2: ^{1}H-NMR spectrum of (*R/S*)-4-methoxy-α-Methylbenzylamine.

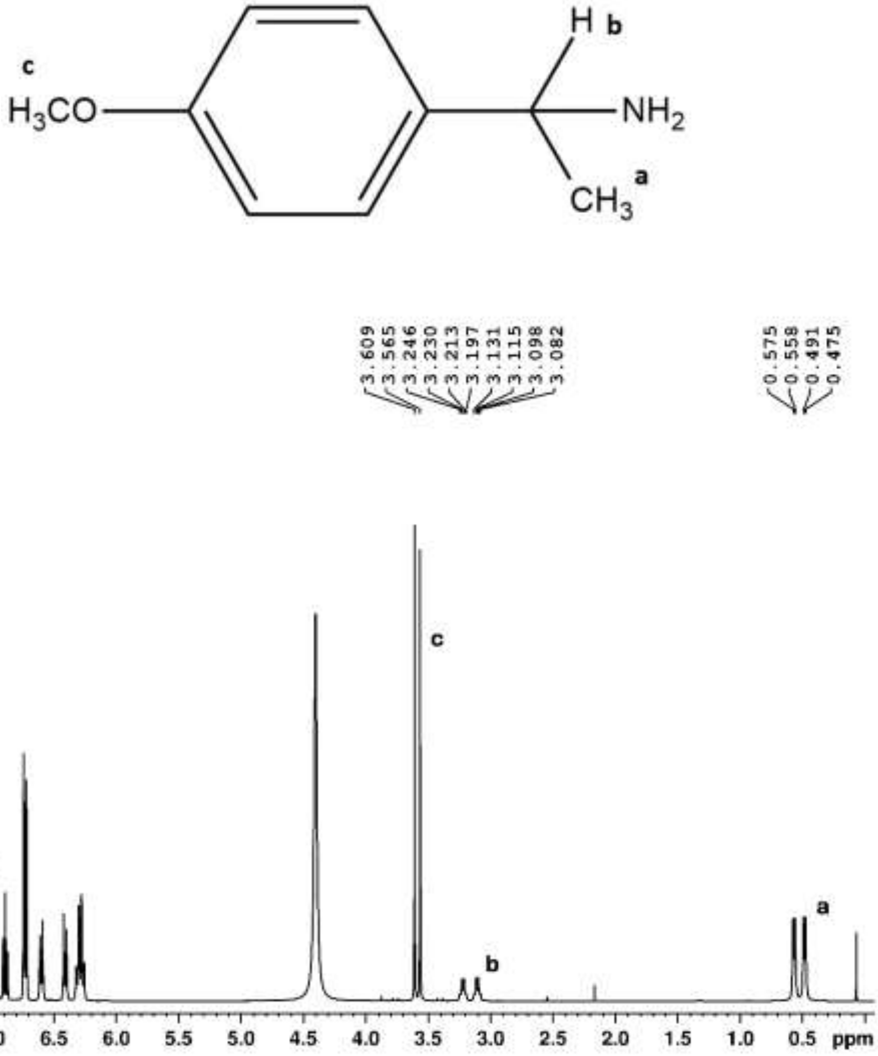


Figure S3: ^{1}H-NMR spectrum of (*R/S*)-4-methyl-α-Methylbenzylamine.

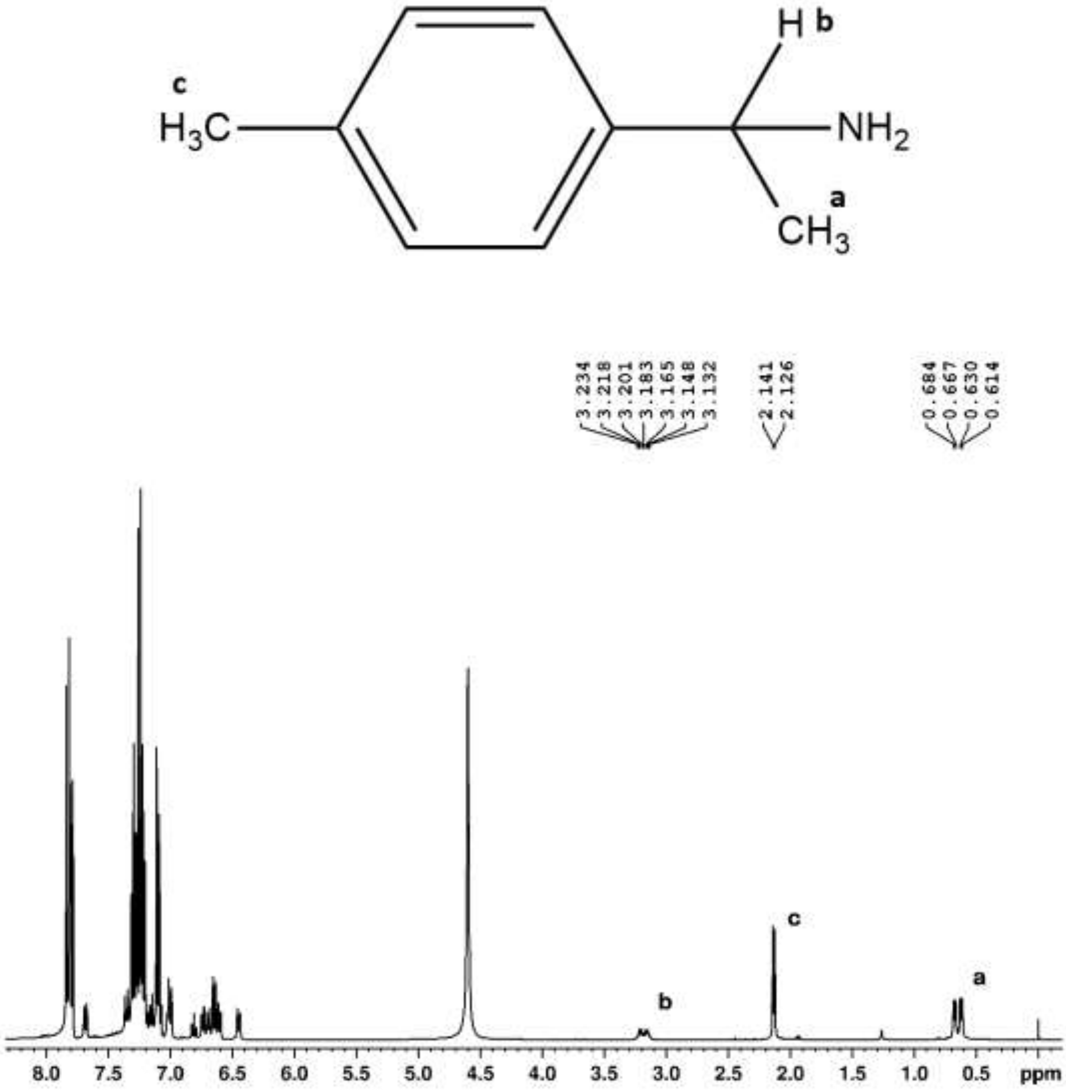


Figure S4: ^{1}H-NMR spectrum of (*R/S*)-*sec*-butylamine.

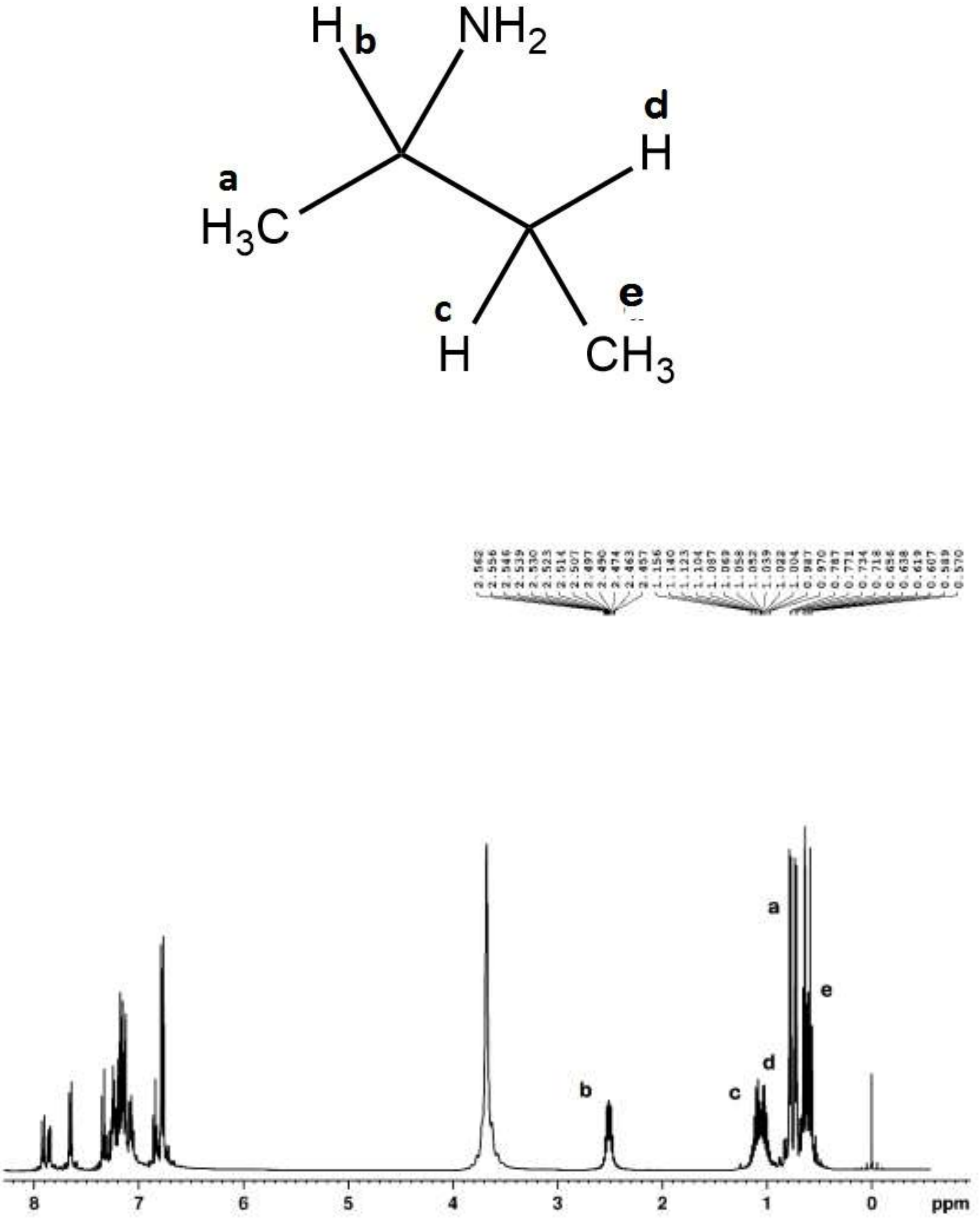


Figure S5: ^{1}H-NMR spectrum of (*R/S*)-α-ethylbenzylamine.

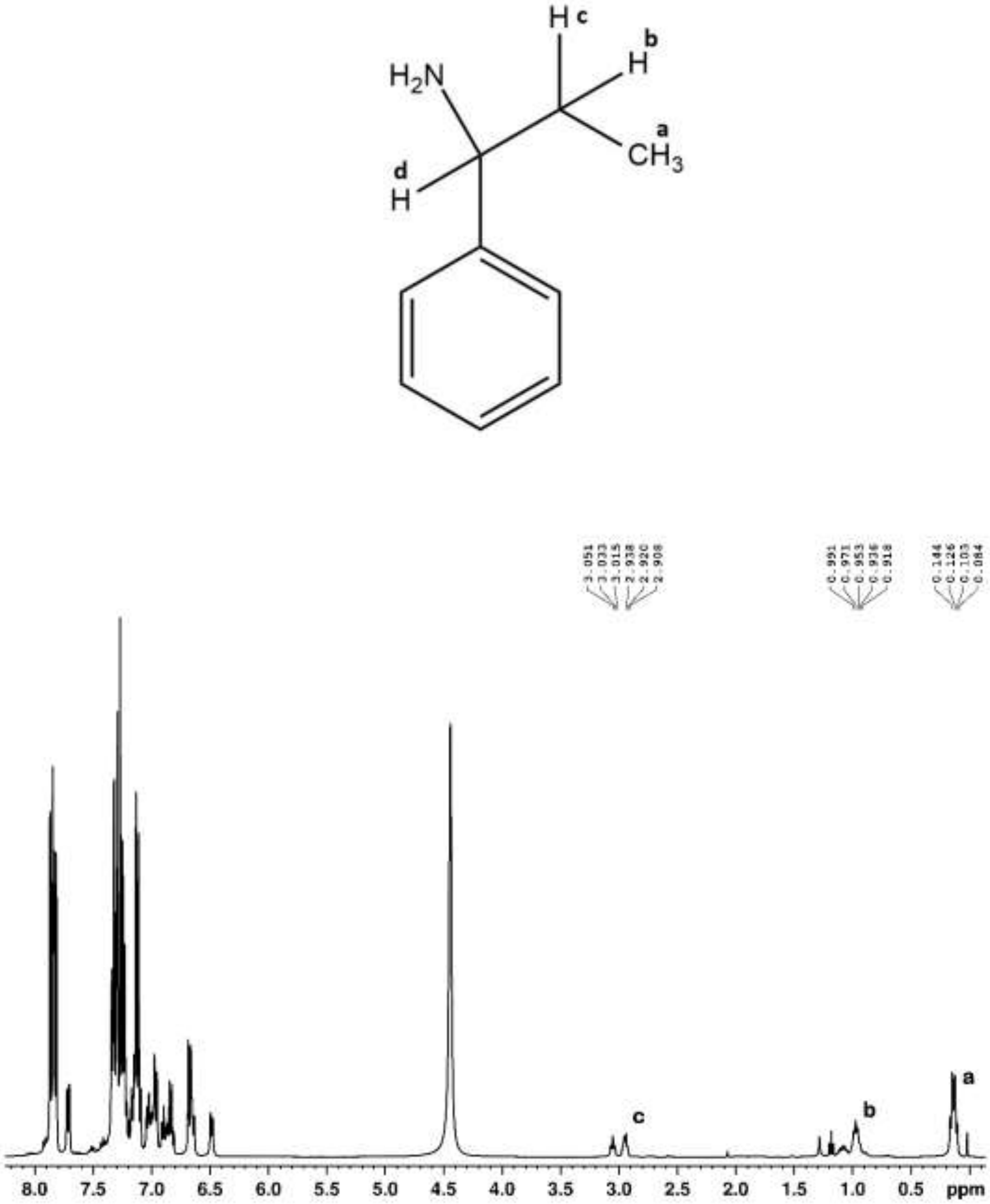
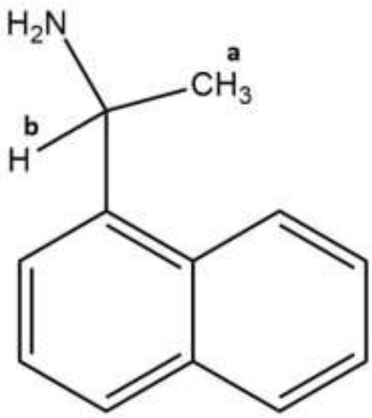


Figure S6: ^{1}H-NMR spectrum of (*R/S*)-α-methylnapthylamine.


H_2N
a
CH_3
b
H

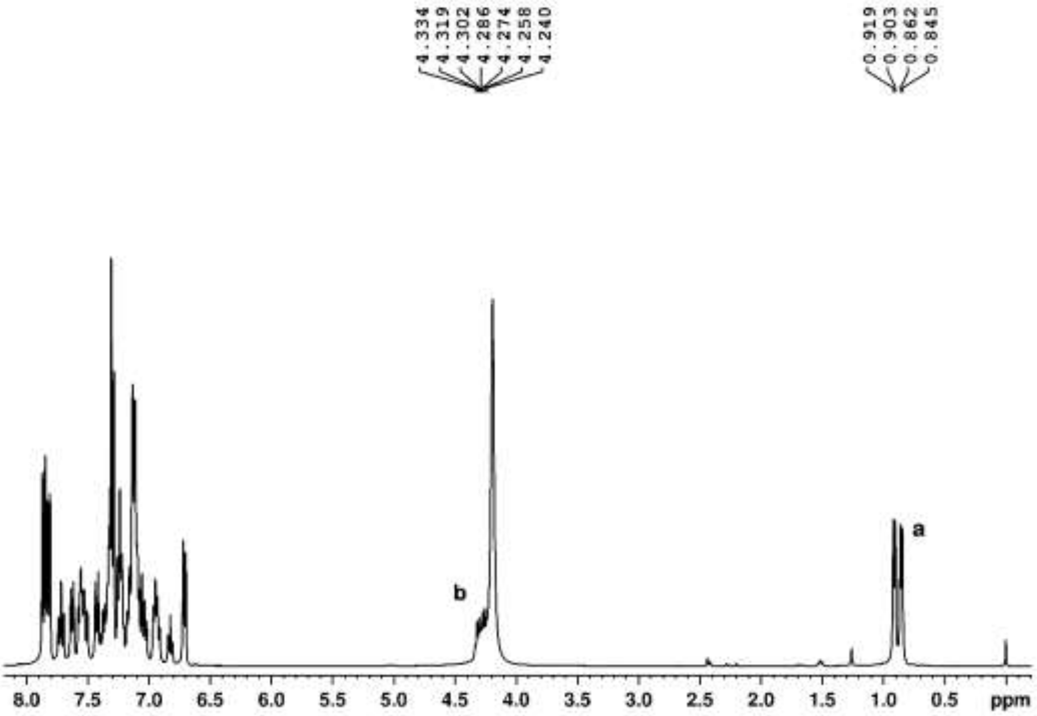

4.334
4.319
4.302
4.286
4.274
4.258
4.240
0.919
0.903
0.862
0.845
b
a
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

Figure S7: ^{1}H-NMR spectrum of (*R/S*)-α-methylbenzylamine.

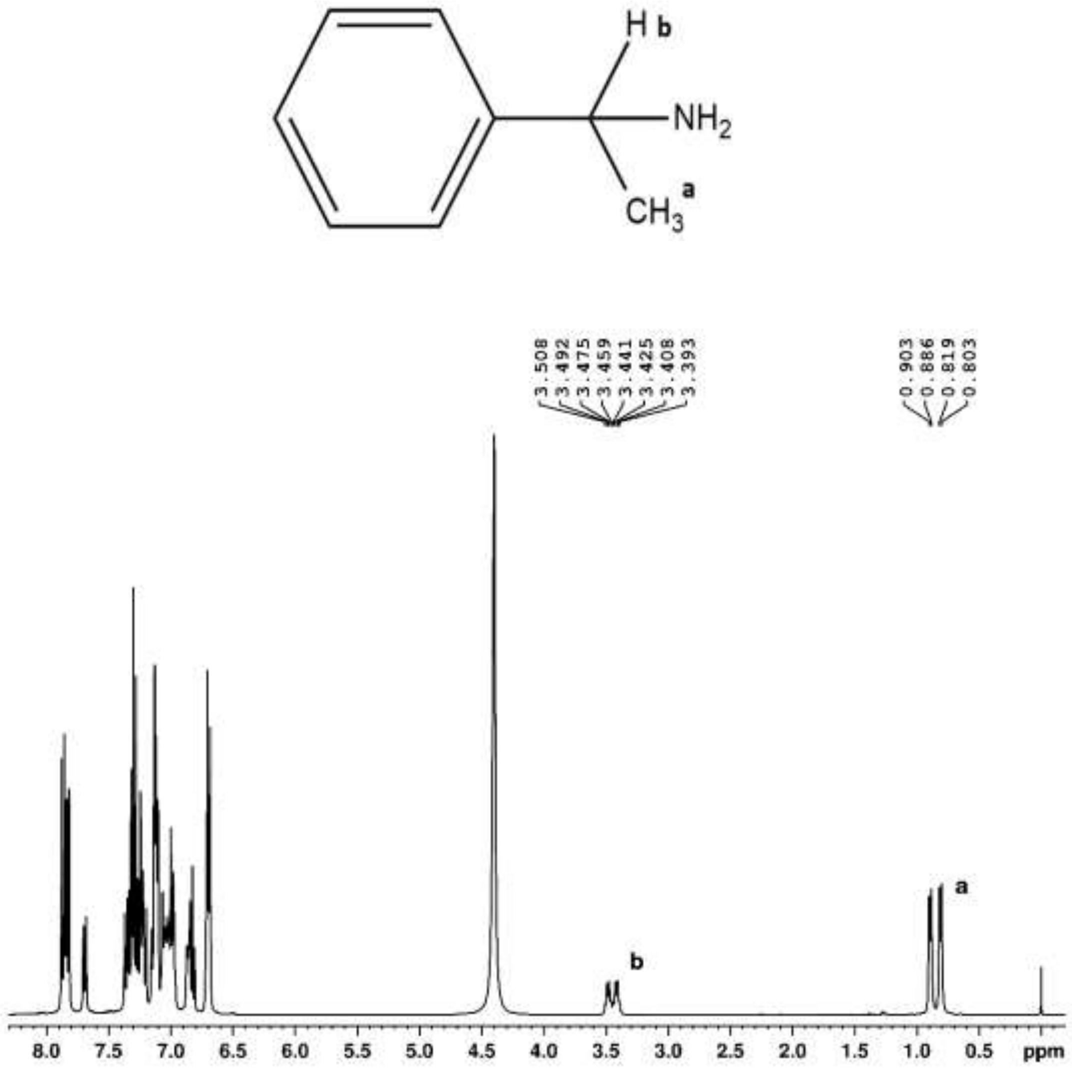


Figure S8: ^{1}H-NMR spectrum of (*R/S*)-1,2-diphenylethyalamine.

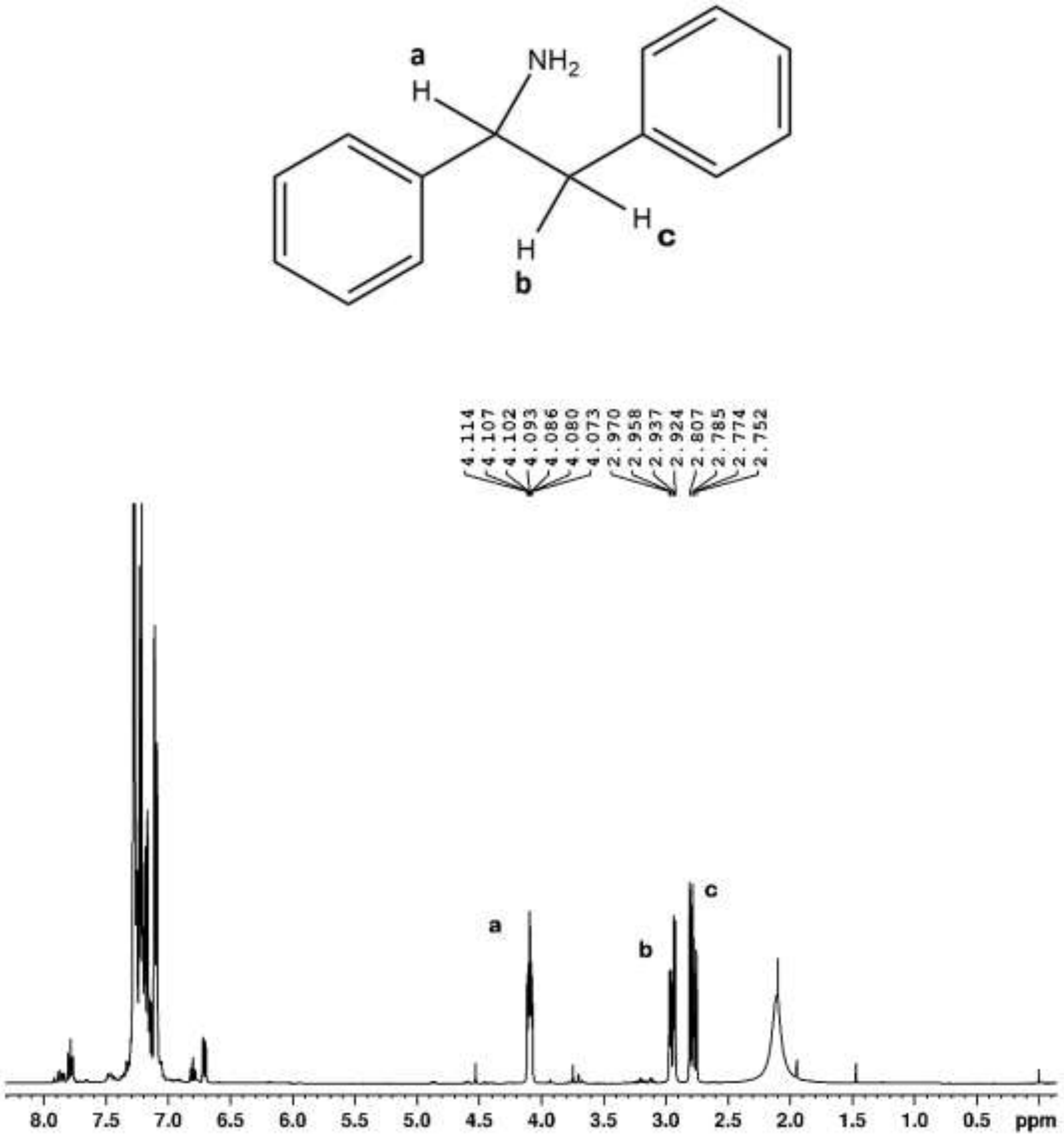


Figure S9: ^{1}H-NMR spectrum of (*R/S*)-1-aminoindane.

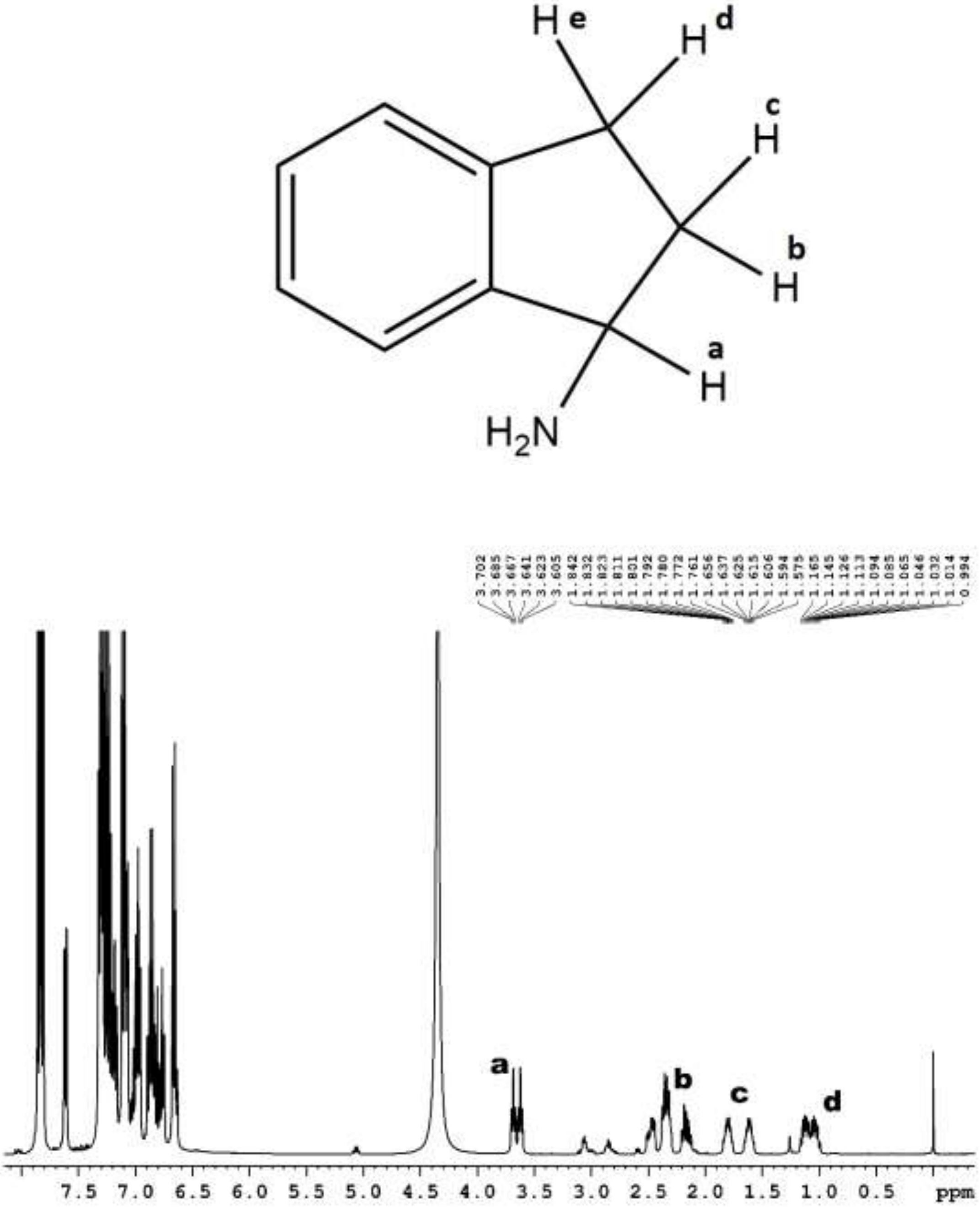
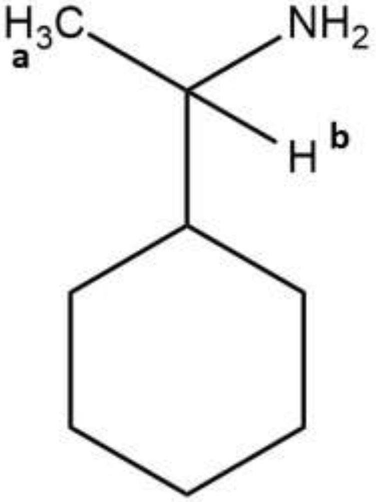


Figure S10: ^{1}H-NMR spectrum of (*R/S*)-1-cyclohexylethylamine.



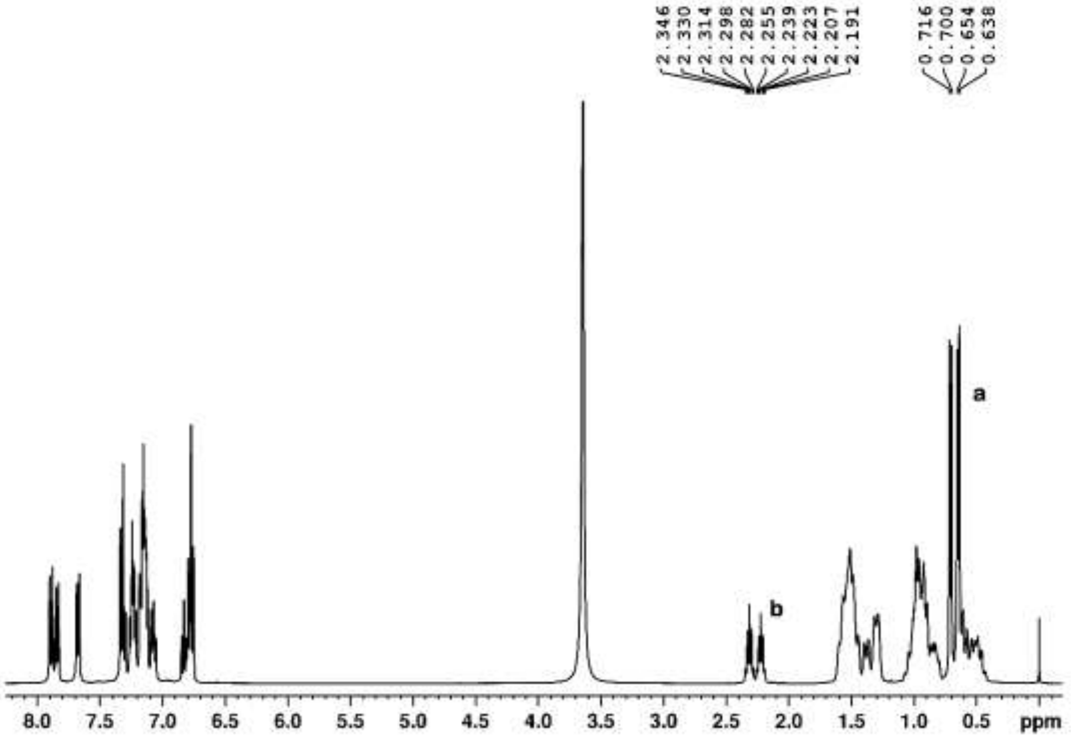


Figure S11: ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine.

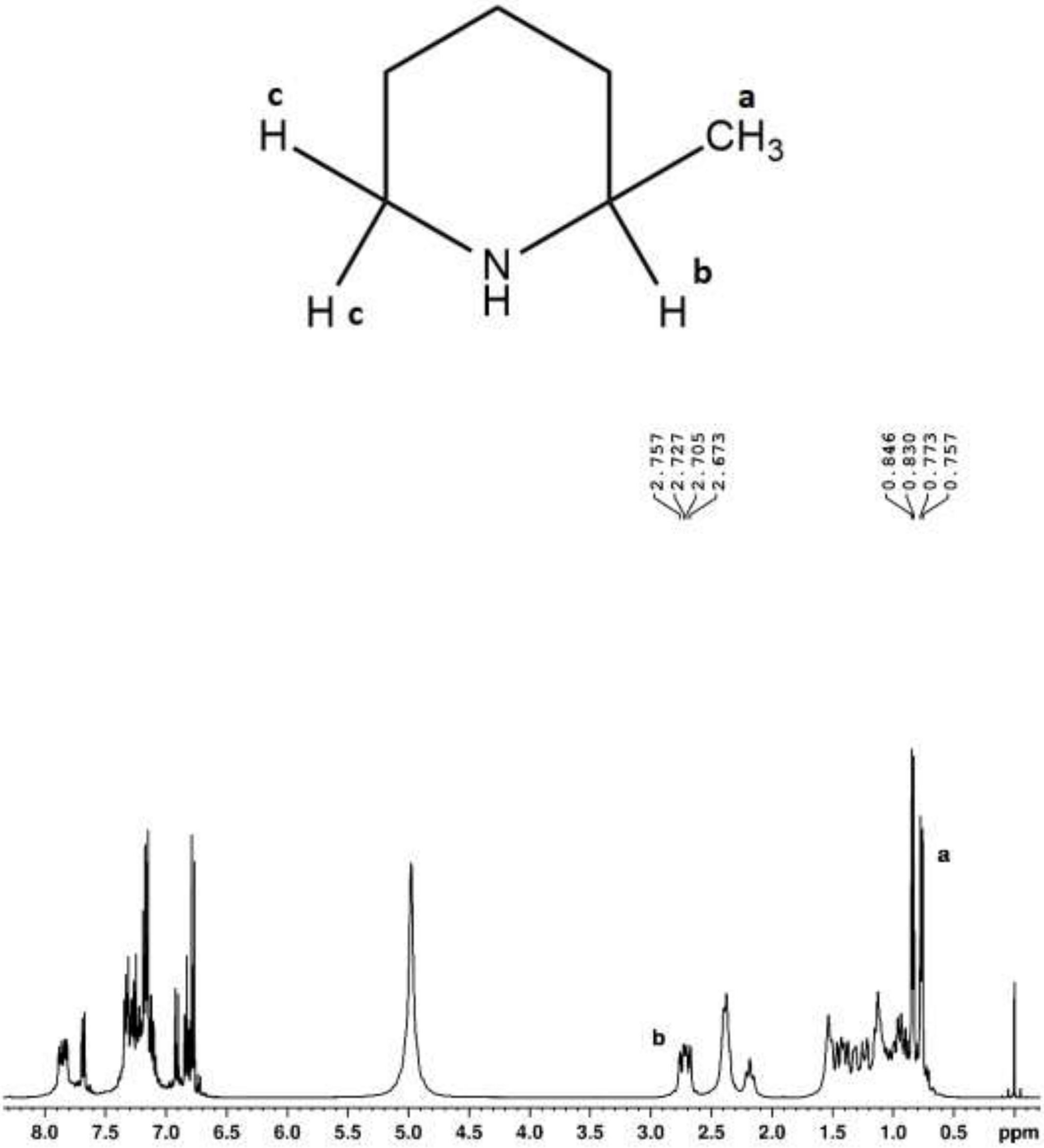


Figure S12: ^{1}H-NMR spectrum of (*R/S*)-N-α-dimethylbenzylamine.

Please note: The differential intensity for CH_3 group is arising because of the formation of salt by one enantiomer. This causes the broadening of the signal. However, the equal integrated intensity confirms, there is no kinetic resolution.

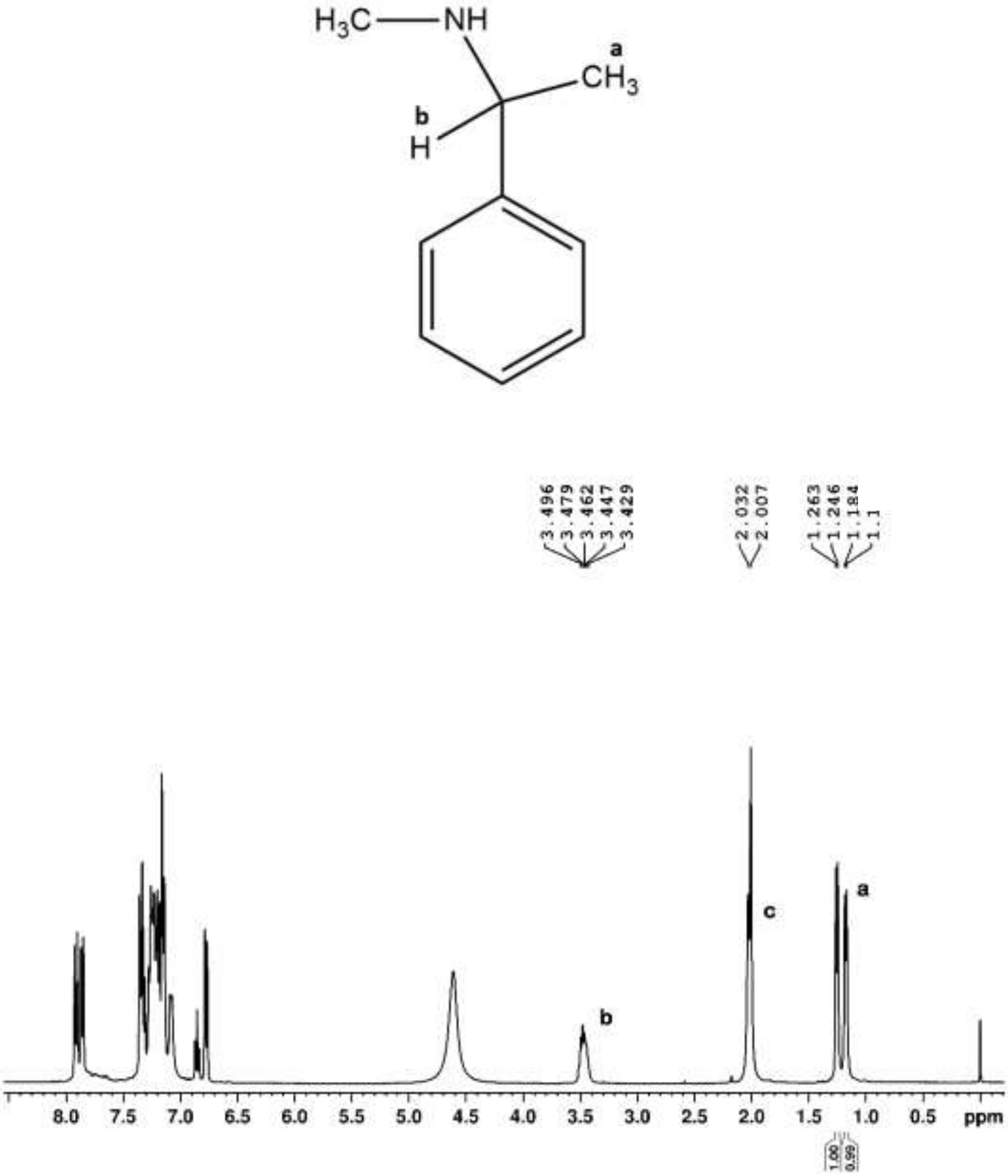


Figure S13: ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperazine.

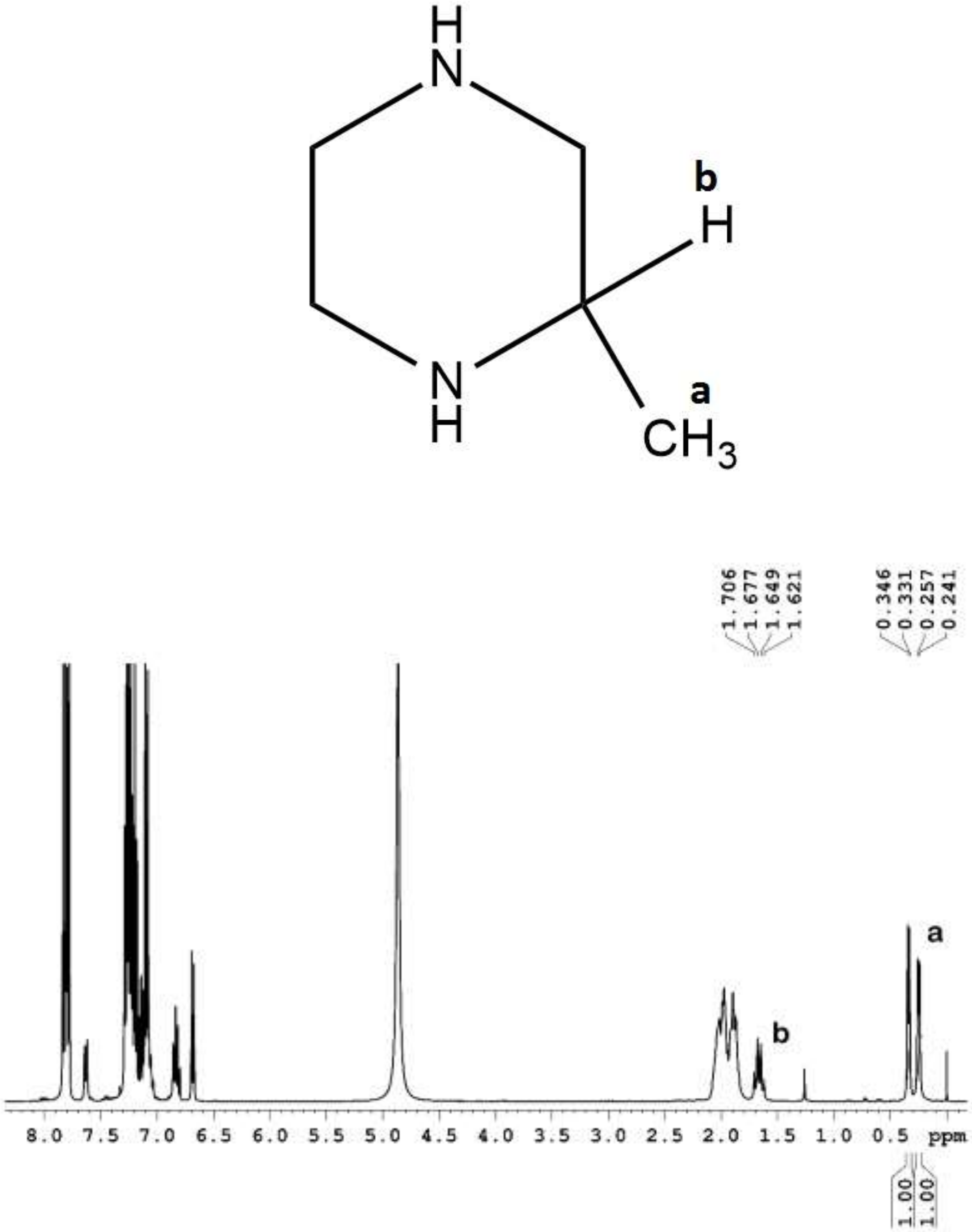


Figure S14: ^{1}H-NMR spectrum of (*R/S*)-ethylpiperidine-3-carboxylate.

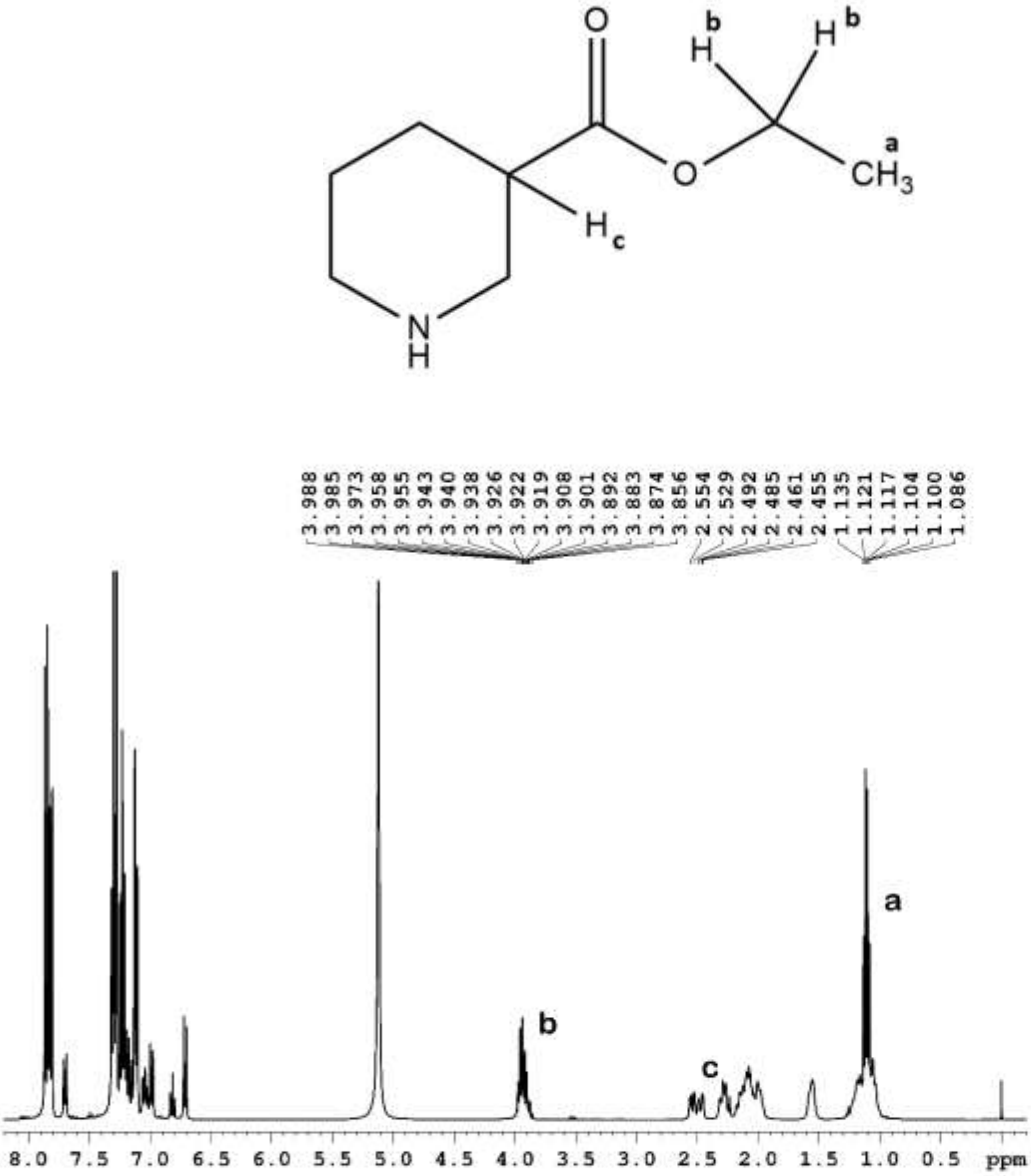


Figure S15: ^{1}H-NMR spectrum of (*R/S*)-N-methyl-1-(-naphthyl)ethylamine.

Please note: The differential intensity for CH_3 group (proton a) is arising because of the formation of salt by one enantiomer. This is confirmed by using enantiopure compound. This causes the broadening of the signal. However, the equal integrated intensity confirms, there is no kinetic resolution.

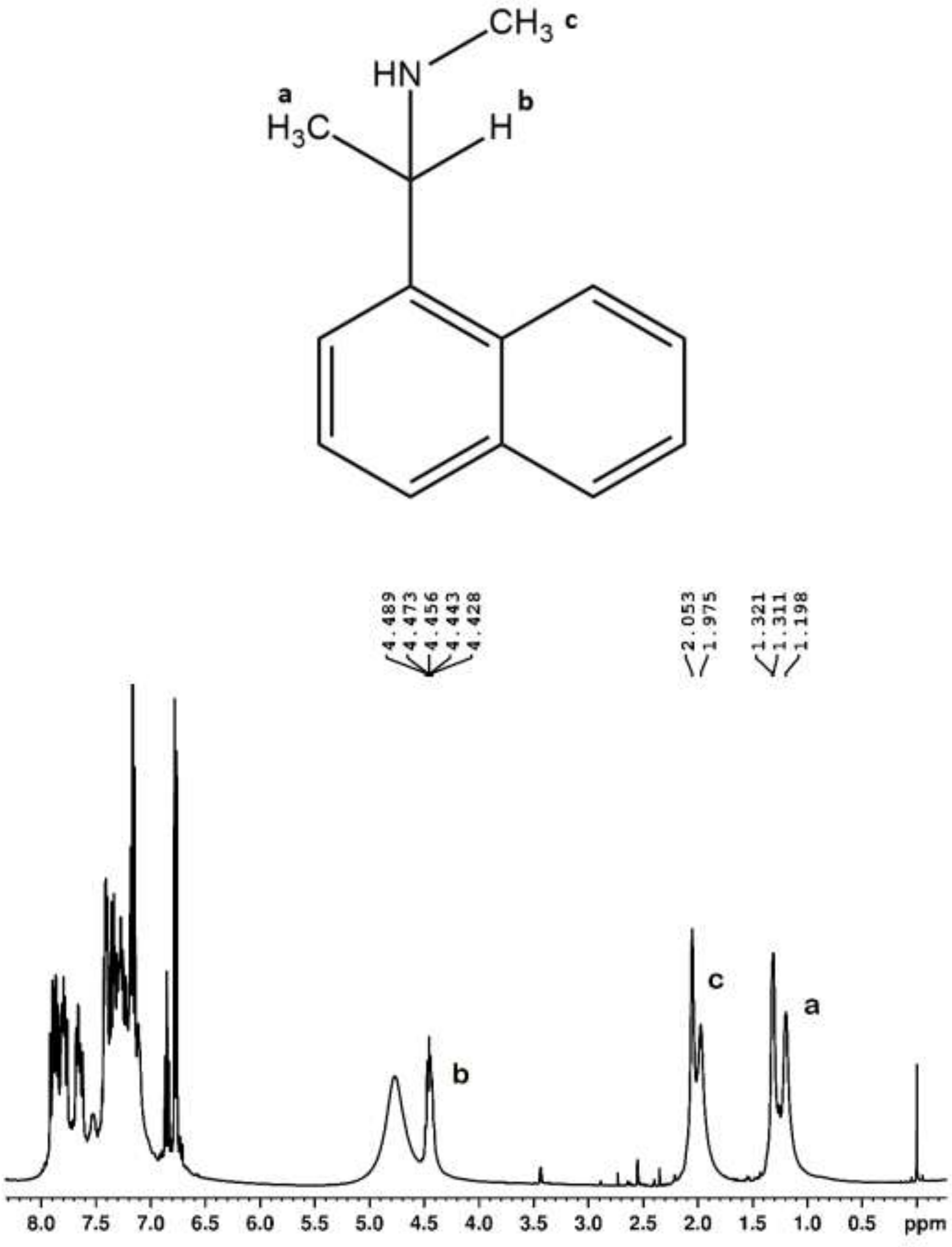


Figure S16: ^{1}H-NMR spectrum of (*R/S*)-N,N-dimethylphenylethylamine.

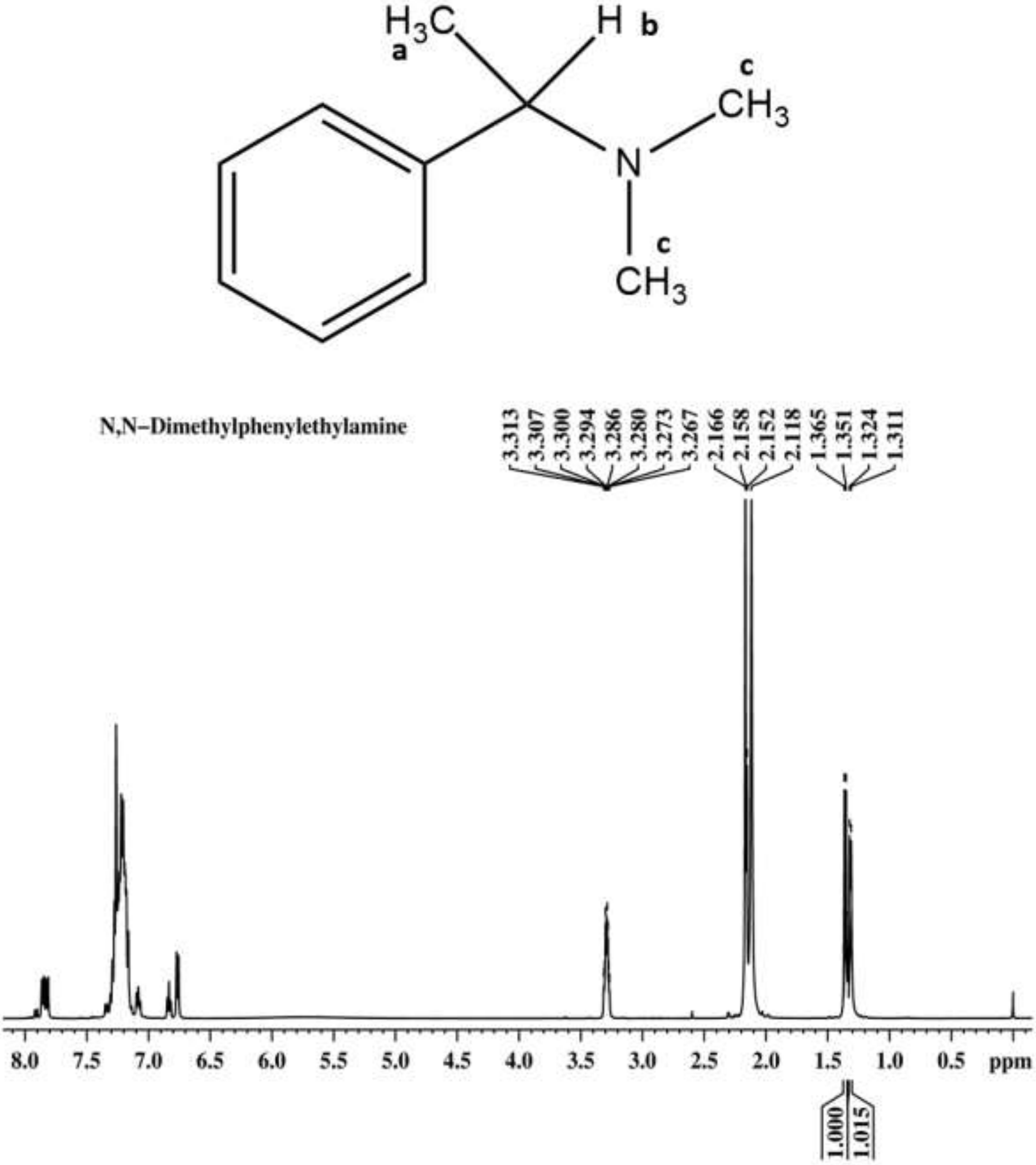


Figure S17: ^{1}H-NMR spectrum of (*R/S*)-2,amino,1,2-diphenylethanol.

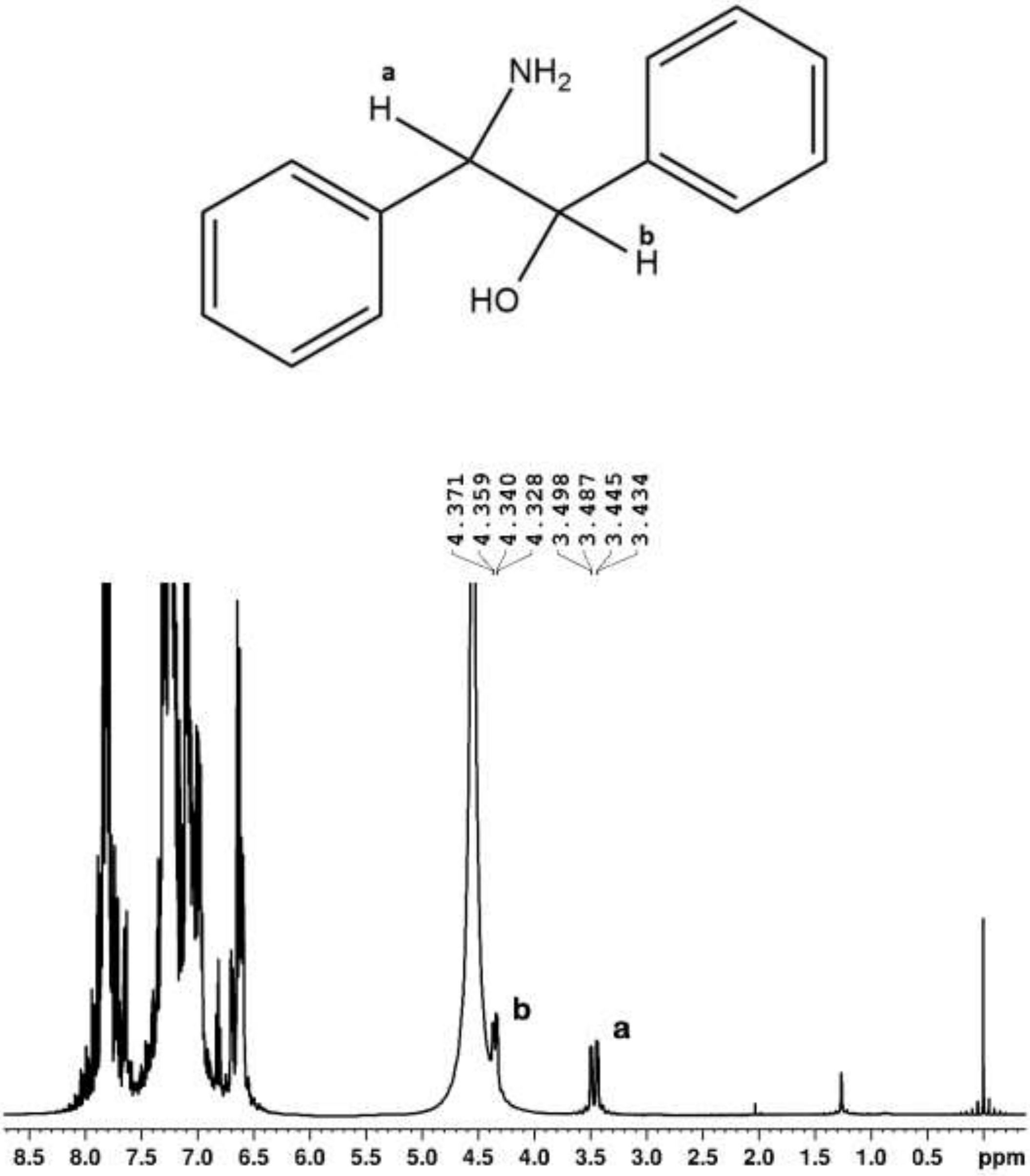


Figure S18: ^{1}H-NMR spectrum of (*R/S*)-2-Phenylglycinol.

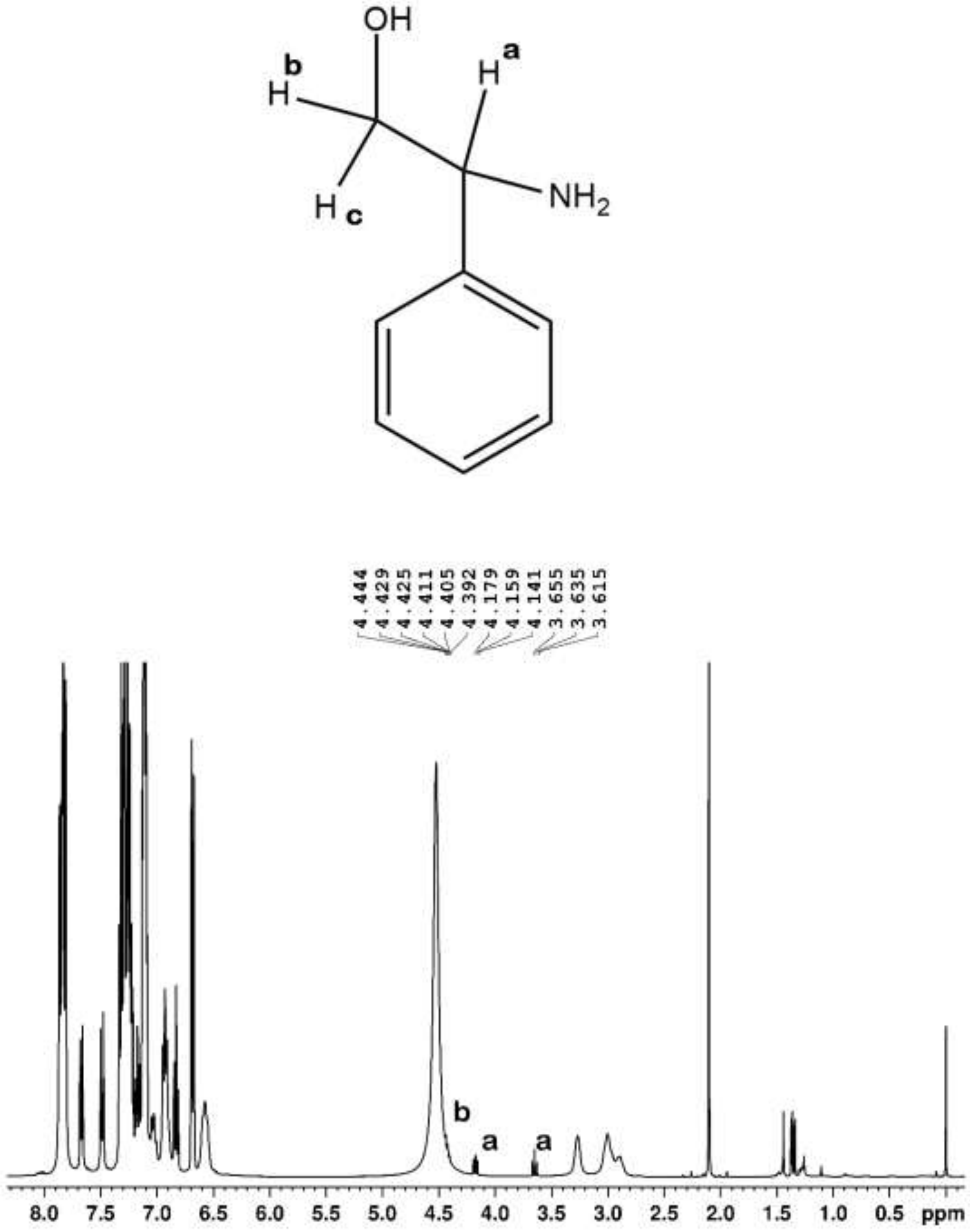
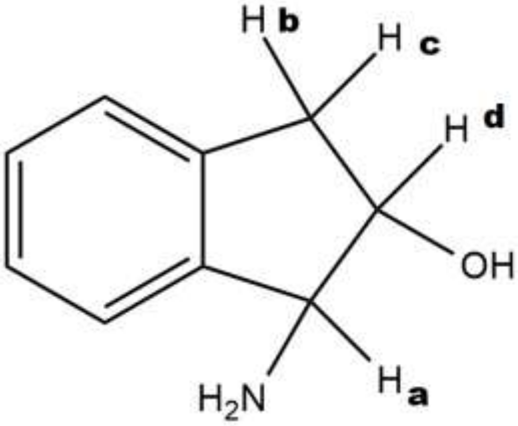


Figure S19: ^{1}H-NMR spectrum of (*R/S*)-1-Amino, 2-indanol.



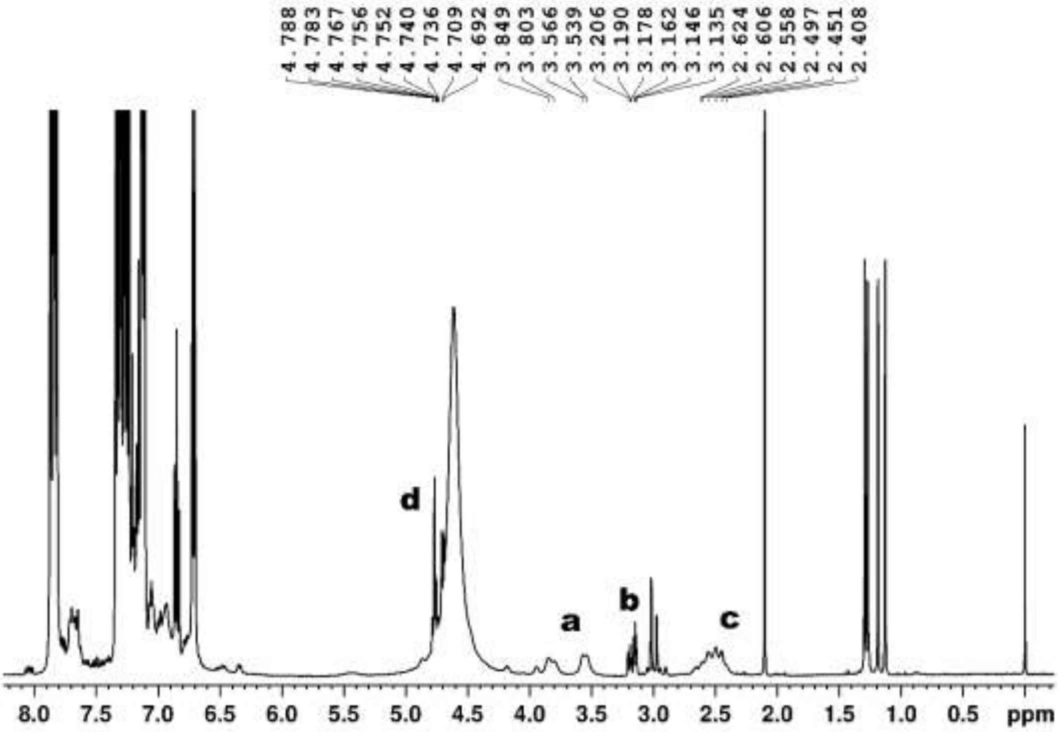


Figure S20: ^{1}H-NMR spectrum of (*R/S*)-2-amino-1-butanol.

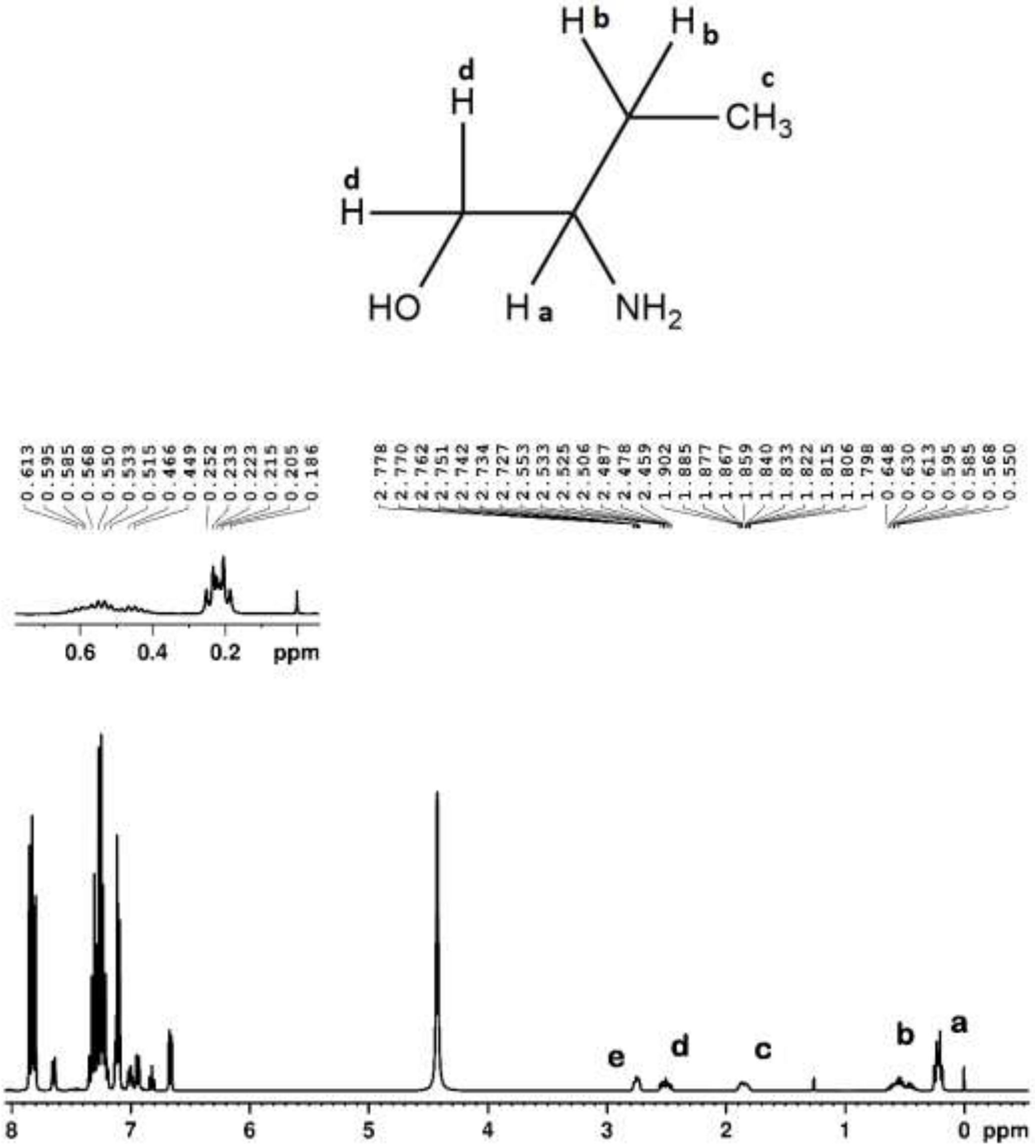


Figure S21: ^{1}H-NMR spectrum of (*R/S*)-α-α-diphenyl-2-pyrrolidinemethanol.

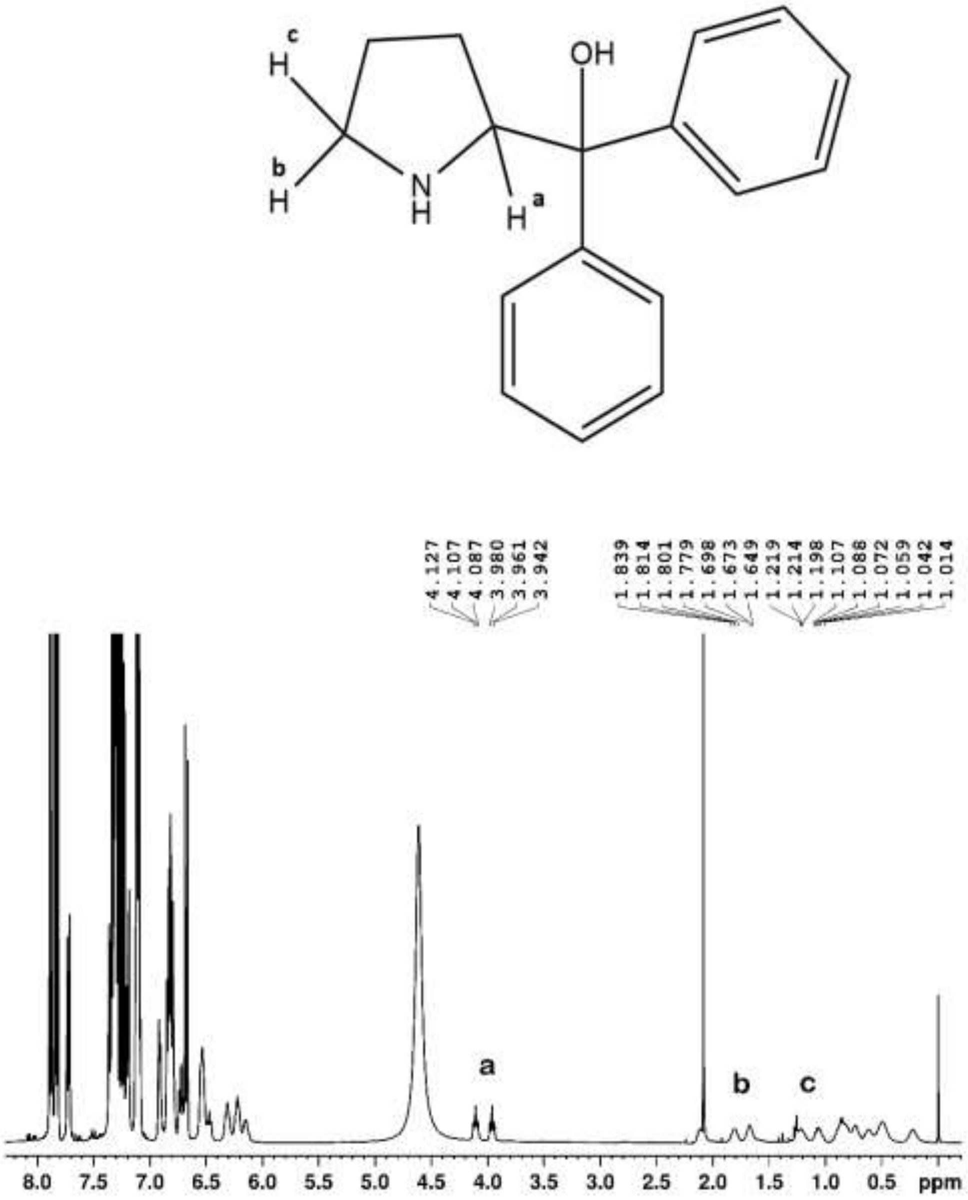


Figure S22: ^{1}H-NMR spectrum of (*R/S*)-2-piperidinemethanol.

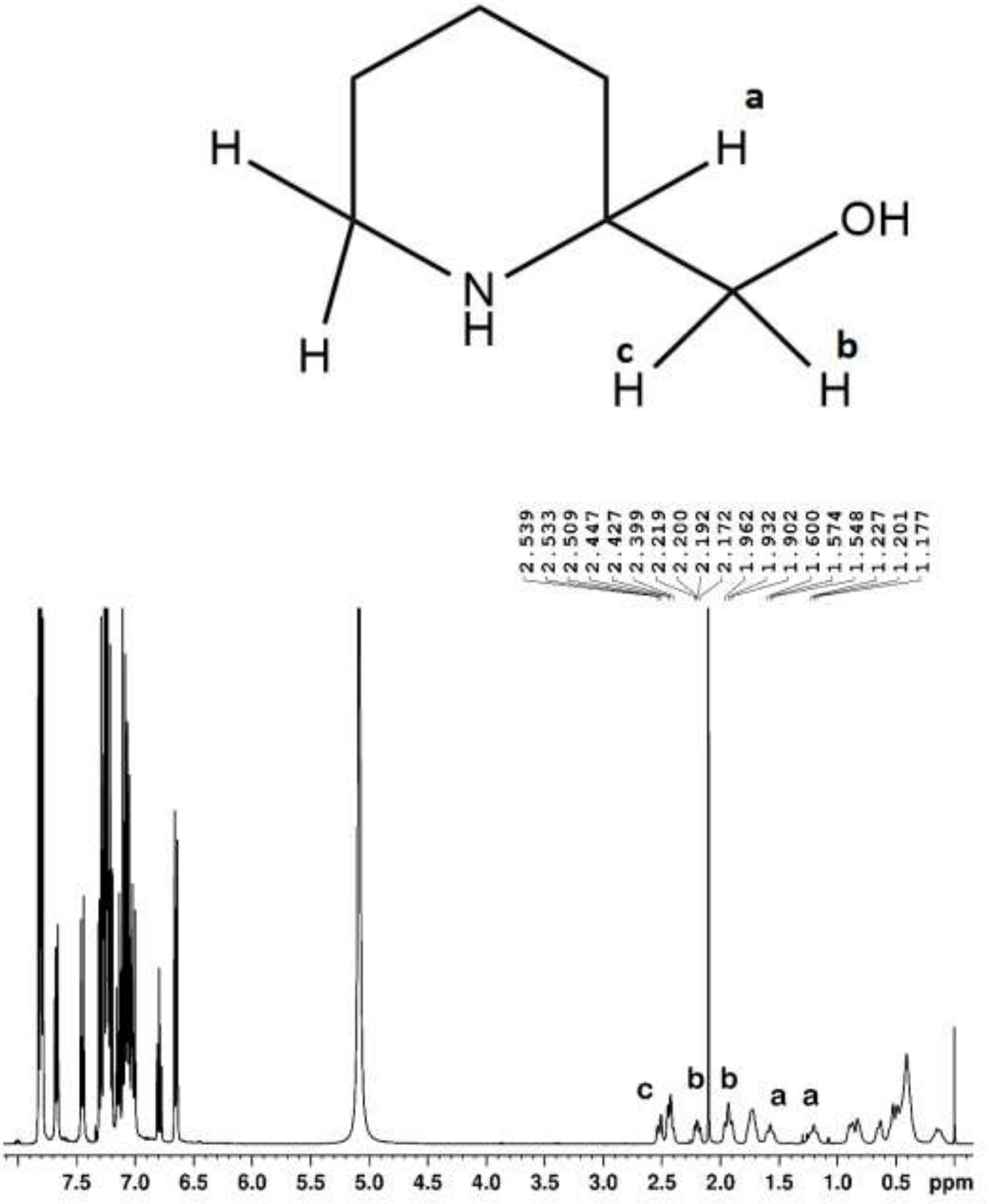


Figure S23: ^{1}H-NMR spectrum of (*R/S*)-2-fluorobenzylamine.

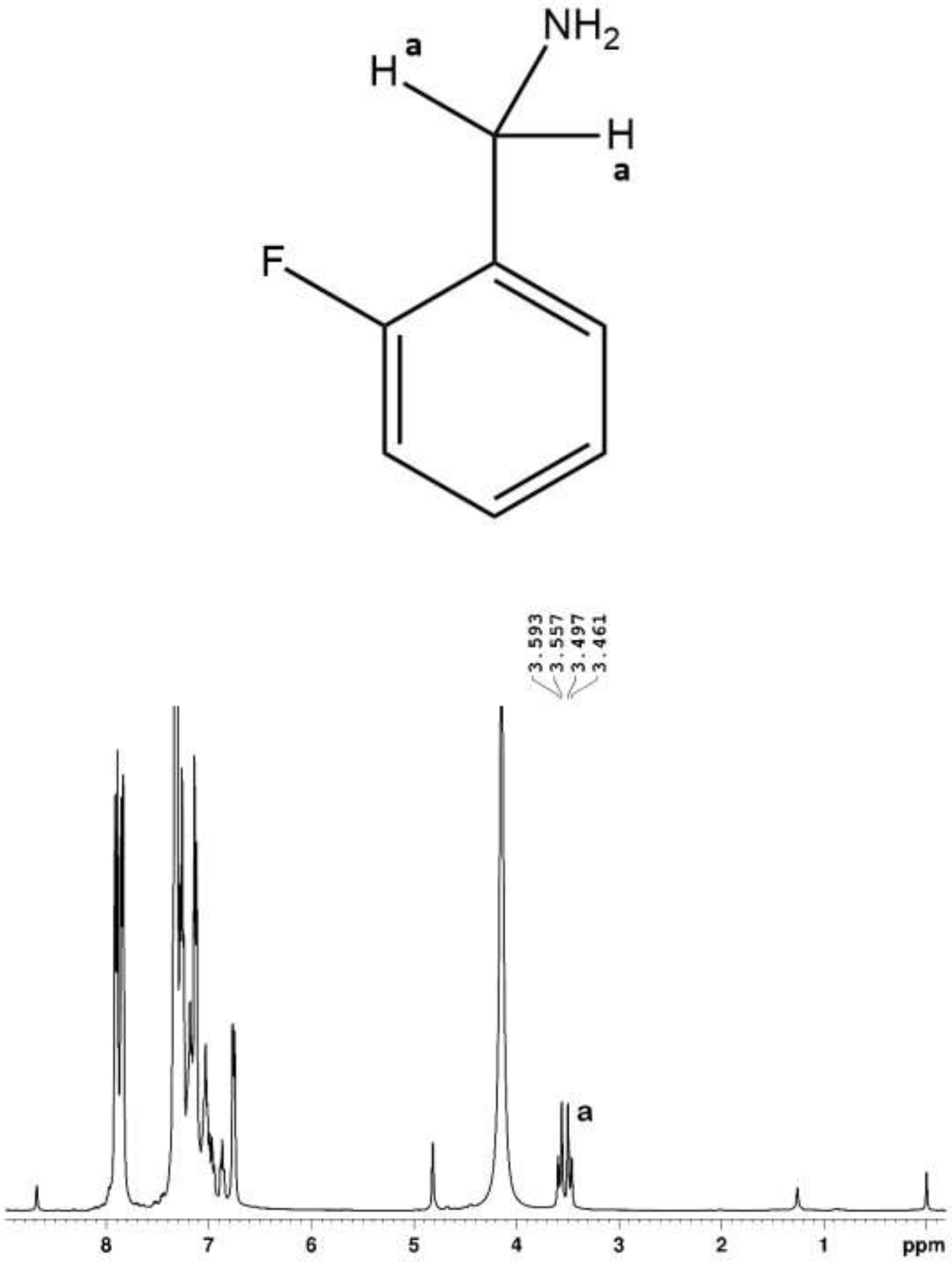


Figure S24: ^{1}H-NMR spectrum of (*R/S*)-benzylamine.

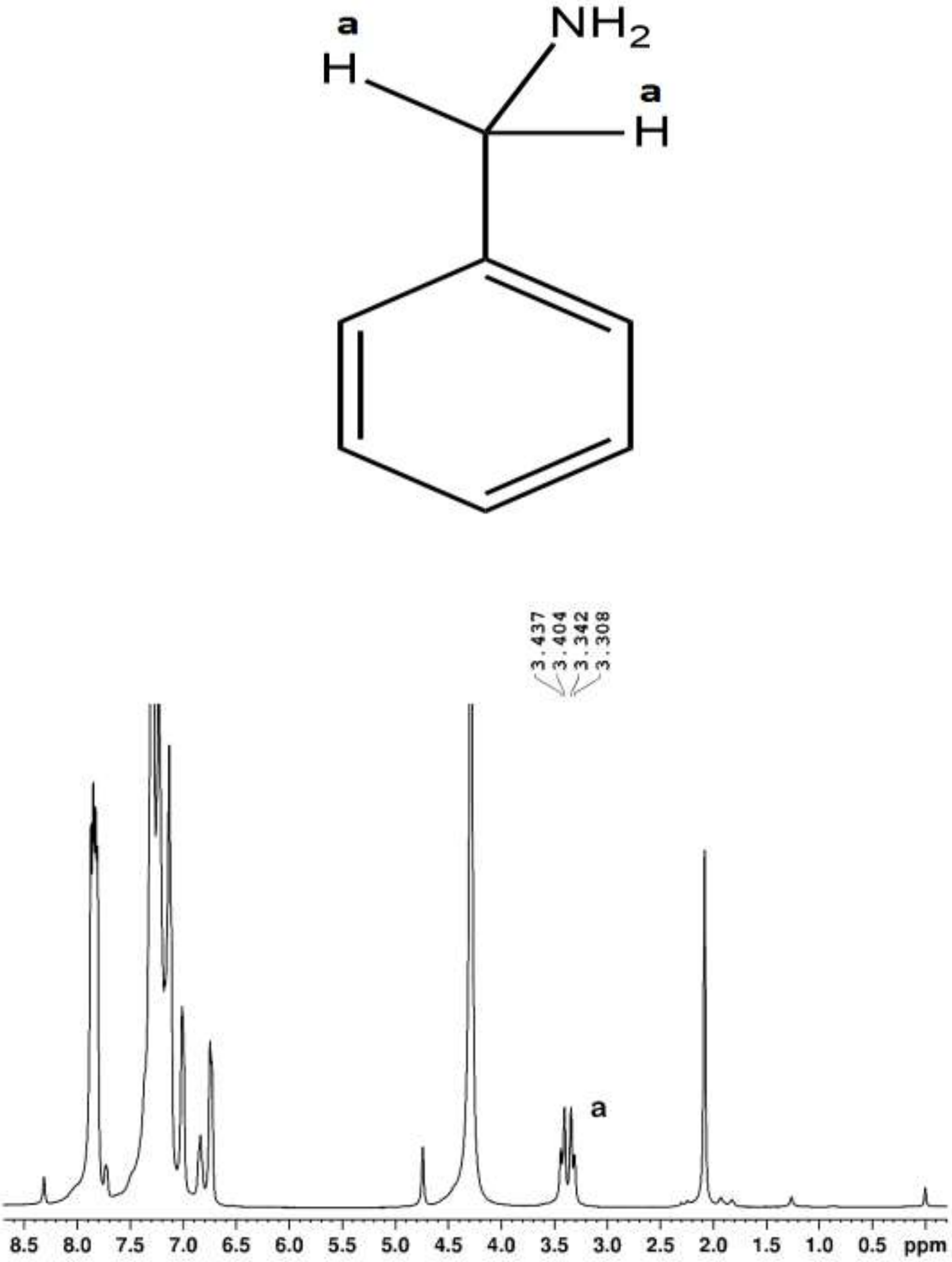


Figure S25: ^{1}H-NMR spectrum of (*R/S*)-isopropylamine.

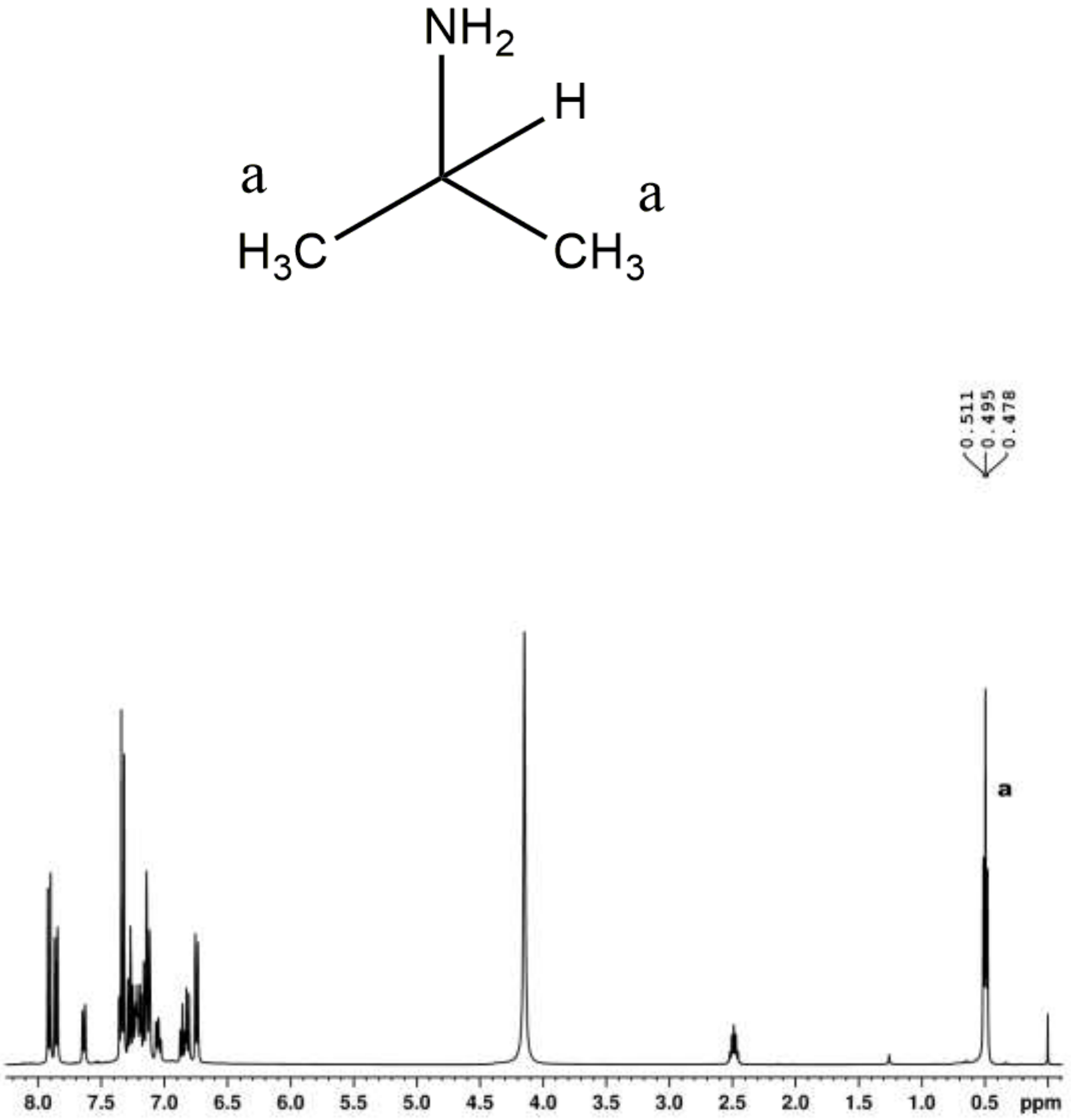


Figure S26: ^{1}H-NMR spectrum of (*R/S*)-2-amino-2-methyl-1-propanol.

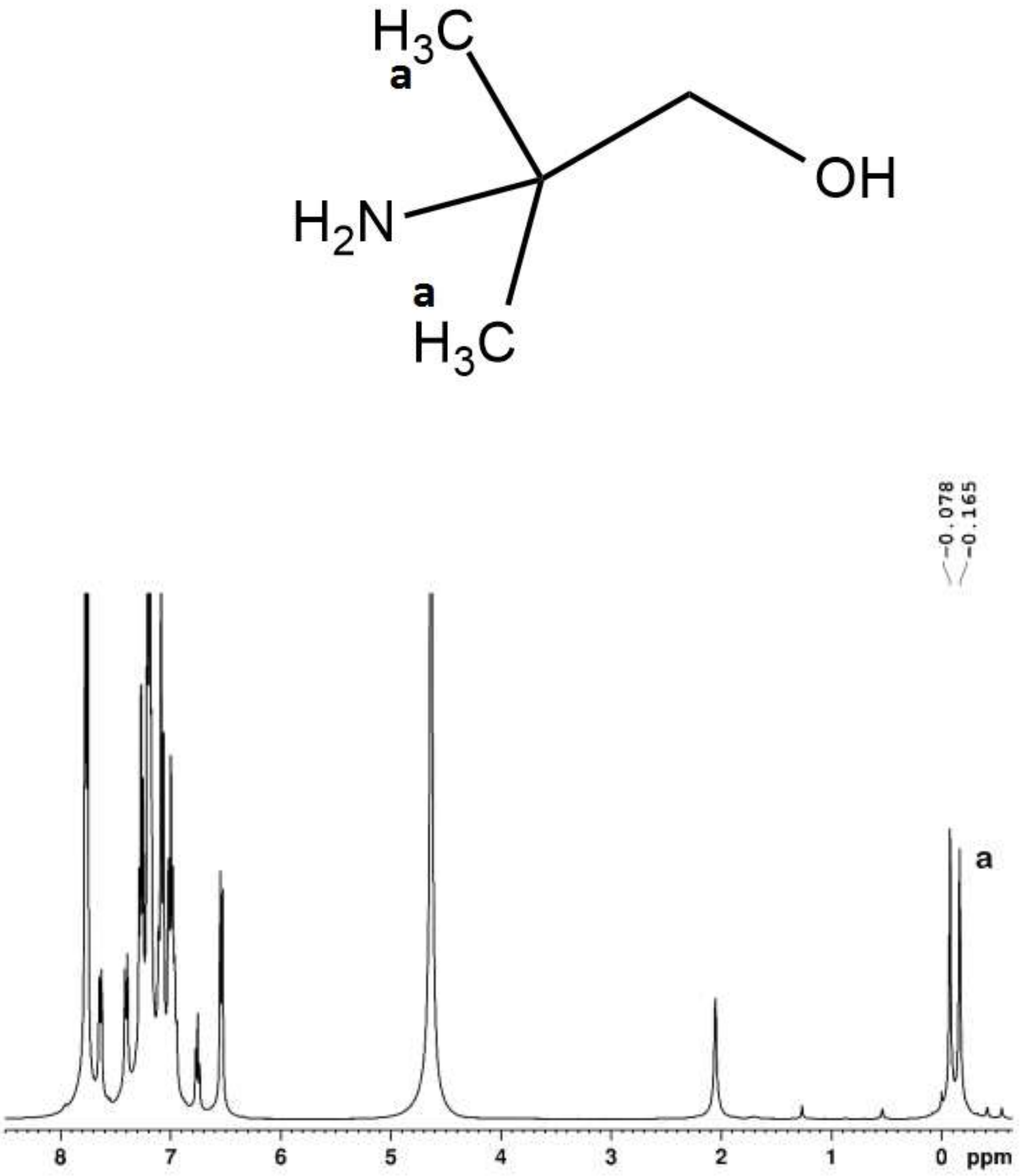
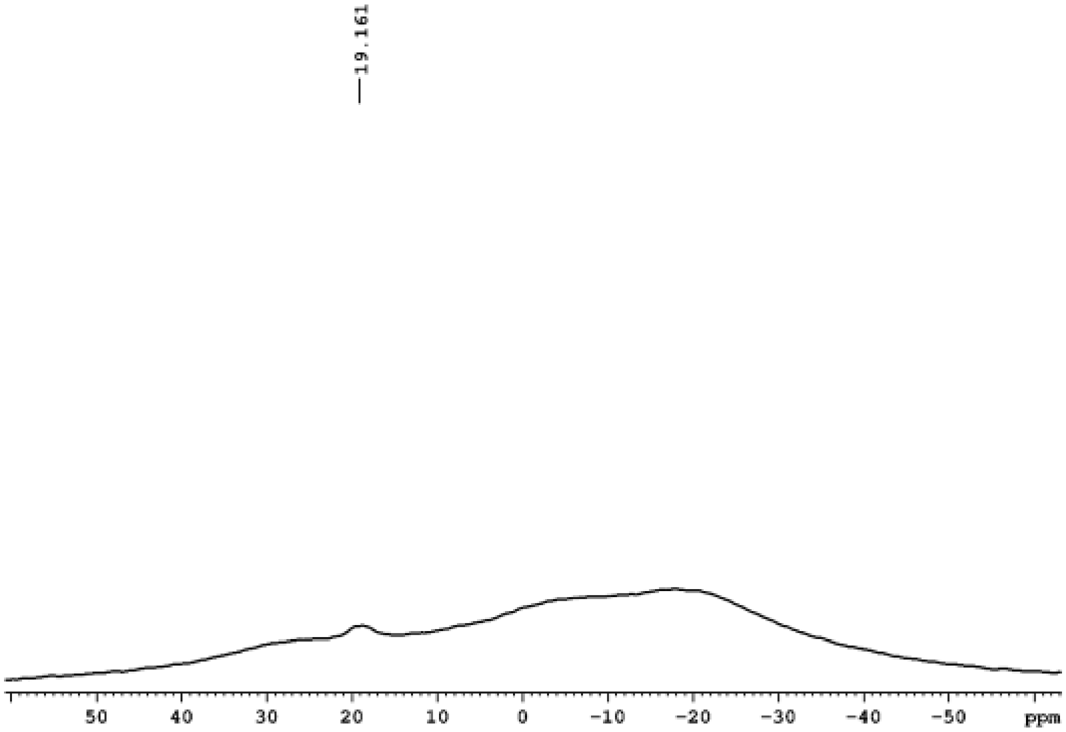
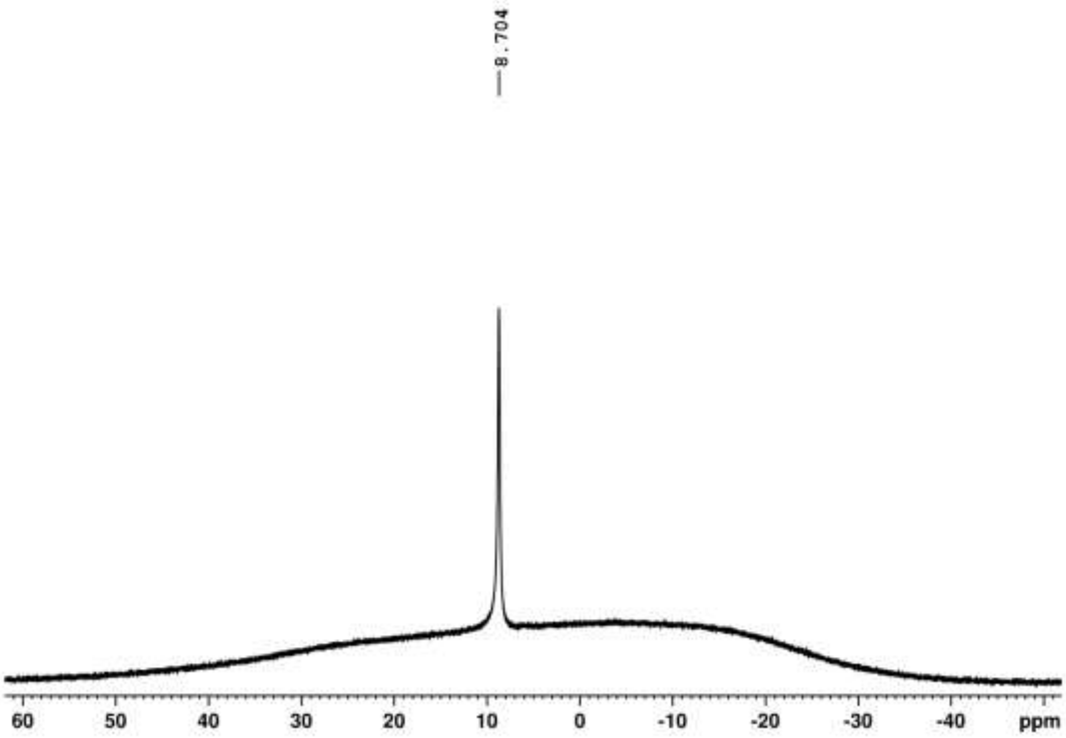


Figure S27: Comparison of ^{11}B NMR spectrum of **top trace:** Triphenyl borate (without complexation) **bottom trace:** boron complexed with *R*-BINOL and chiral amine at the optimum condition of amine. Peak around at 8 ppm indicating the formation of a tetragonal boronate species. And it is more intense at the optimum condition




8.704
60
50
40
30
20
10
0
-10
-20
-30
-40
ppm

.