Supporting Information

A Versatile Ternary Ionic Complex for Chiral Discrimination of Molecules of Diverse Functionality Using ^{1}H NMR

Indrani Pal, Sachin Rama Chaudhuri, Nagarajarao 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 8022933300, 919845124802

Fax: 0091 8023601550

Index

S23: 45^0 skew projected 2D *J*-resolved spectra of (*R/S*)-2-piperidinemethanol in *R*-BNPA and DMAP

S24: 45^0 skew projected 2D *J*-resolved spectra of (*R/S*)-2-amino-2-phenylethanol in *R*-BNPA and DMAP

S25: 45^0 skew projected 2D *J*-resolved spectra of (*R/S*)-atenolol in *R*-BNPA and DMAP

S26: 45^0 skew projected 2D *J*-resolved spectra of (*R/S*)-2-aminobutanol in *R*-BNPA and DMAP

S27: 45^0 skew projected 2D *J*-resolved spectra of (*R/S*)- 1-chloro-2-propanolnol in *R*-BNPA and DMAP

S28: 45^0 skew projected 2D *J*-resolved spectrum of (*R/S*)-4-phenyl oxazolidine-2-thione in *R*-BNPA and DMAP

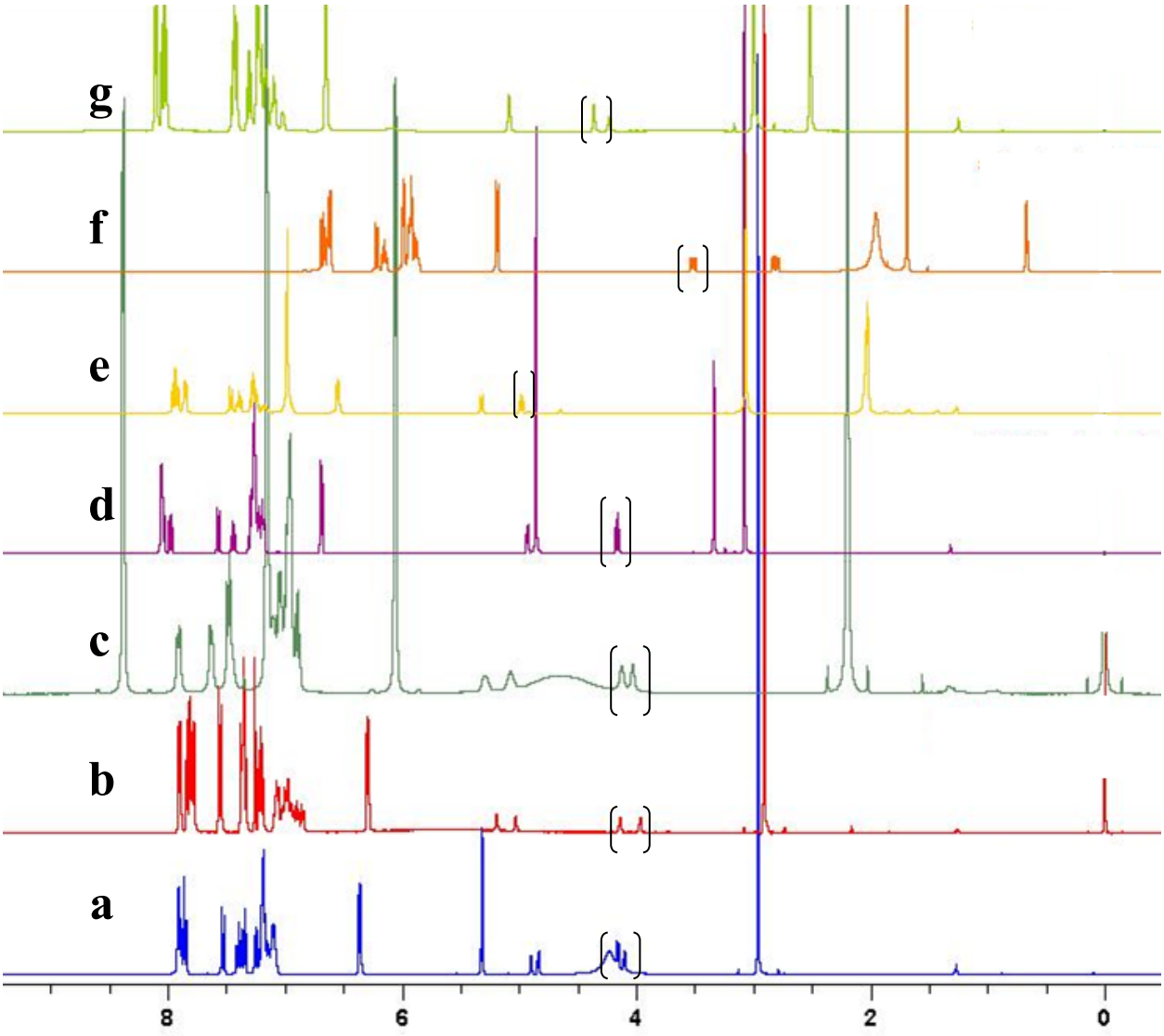
S29: ^{31}P-NMR spectrum of racemic 2-aminobtanol in *R*-BNPA and DMAP

S30: (a) ^{31}P-NMR spectrum of R-2-aminobtanol in *R*-BNPA and DMAP and (b) ^{31}P-NMR spectrum of S-2-aminobtanol in in *R*-BNPA and DMAP

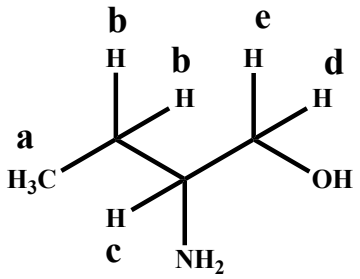
Experimental

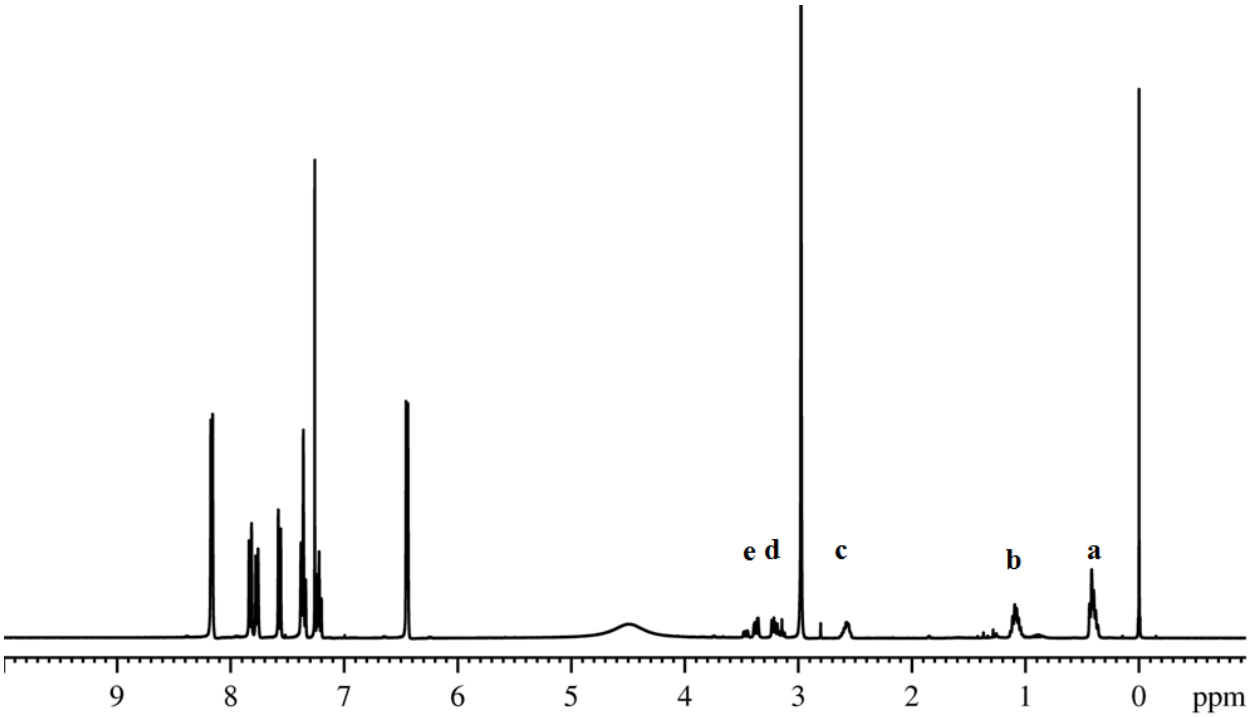
All the chemicals were purchased from Sigma Aldrich and used as received. The ^{1}H NMR experiments were carried out using the Bruker AV-III 400 NMR spectrometer equipped with a TXI probe. The ^{1}H NMR spectra of a series of chiral amino alcohols were obtained using a 1:1 molar mixture of optically pure 1,1'-binapthyl phosphoric acid(BNPA) and DMAP in the solvent $CDCl_3$ at room temperature. The chemical shifts were measured using TMS as an internal reference.

^{1}H NMR spectra of cis-racemic 2-amino-1, 2-diphenyl ethanol in; a) CD_2Cl_2, b) $CDCl_3$, c) C_6D_6, d) CD_3OD, e) CD_3COCD_3, f) CD_3CN and g) DMSO with DMAP. The discriminated peaks are shown in enclosed parenthesis.

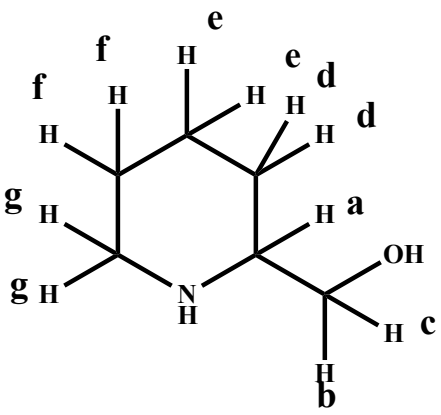


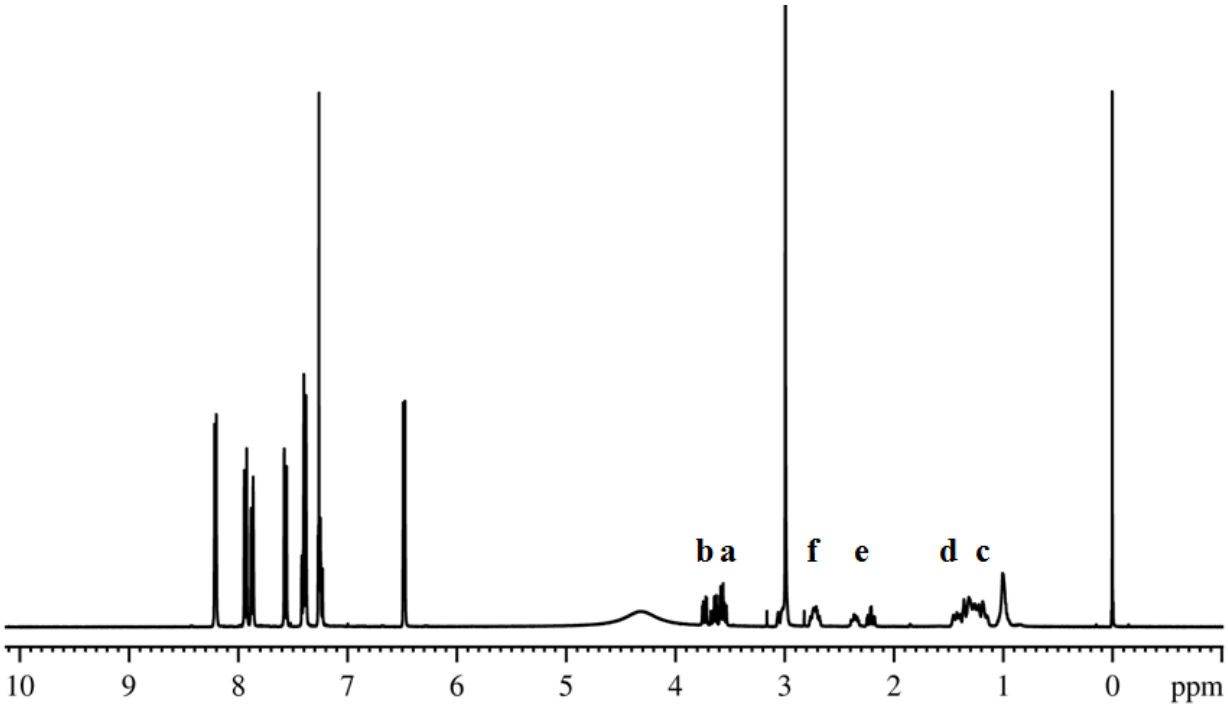
^{1}H-NMR spectrum of (*R/S*)-2-aminobutanol in *R*-BNPA and DMAP



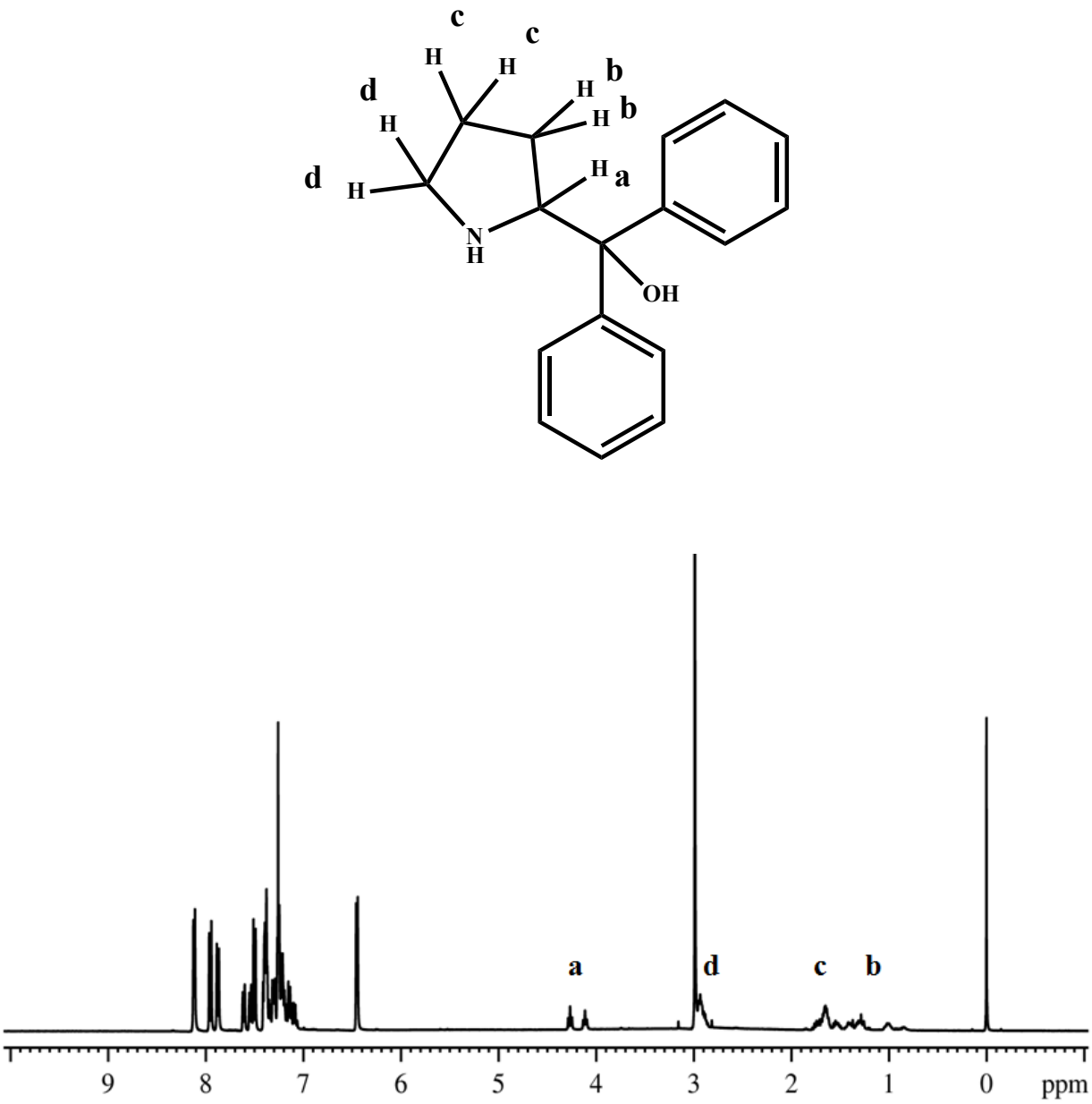


^{1}H-NMR spectrum of (*R/S*)-2-Piperidinemethanol in *R*-BNPA and DMAP

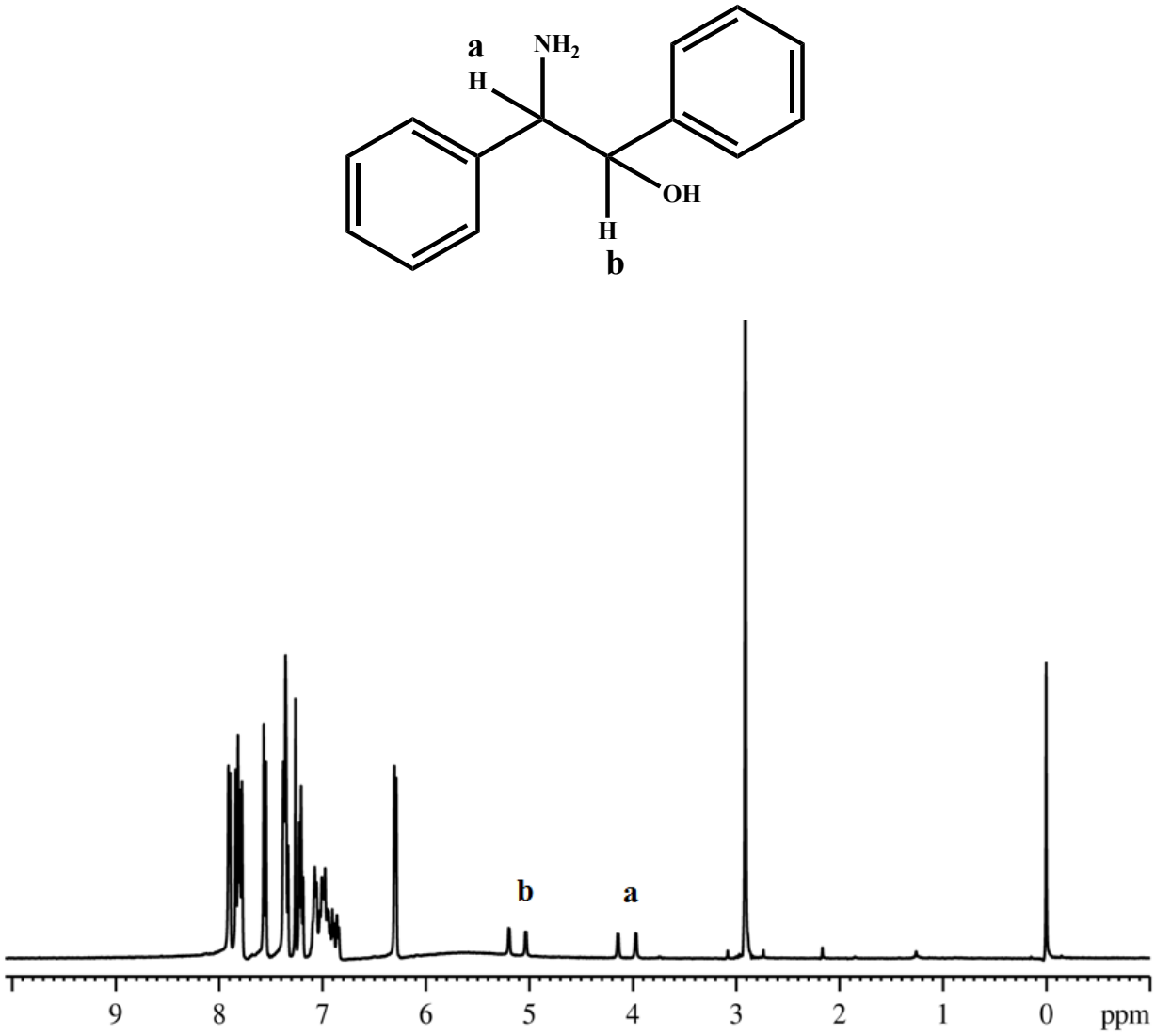




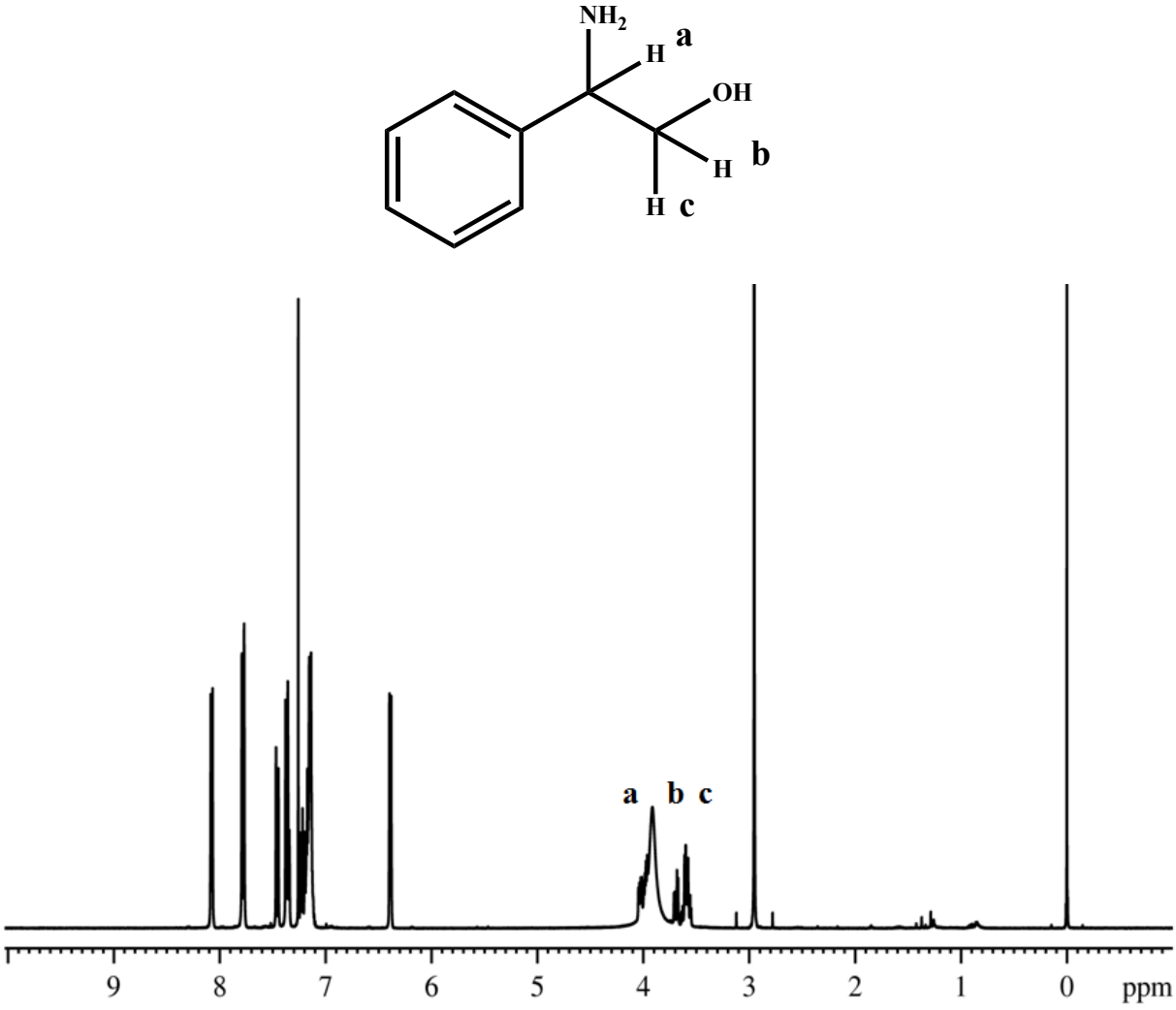
^{1}H-NMR spectrum of (*R/S*)-*α*,*α*-diphenyl-2-pyrrolidinemethanol in *R*-BNPA and DMAP



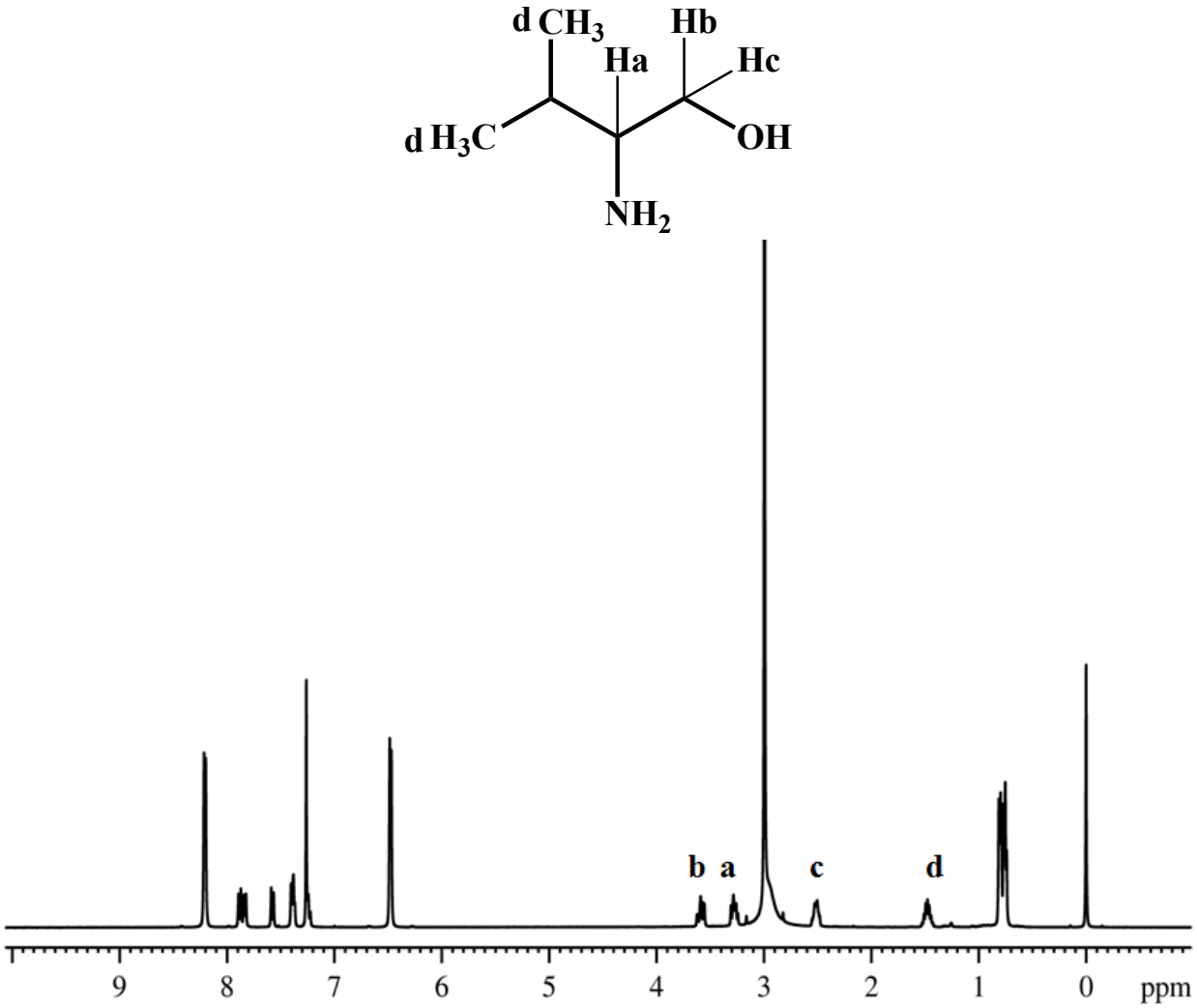
^{1}H-NMR spectrum of (*R/S*)-2-amino-1,2-diphenylethanol in *R*-BNPA and DMAP



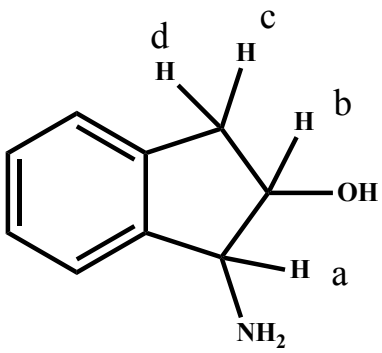
[1]H-NMR spectrum of (*R/S*)-2-amino-2-phenylethanolin *R*-BNPA and DMAP

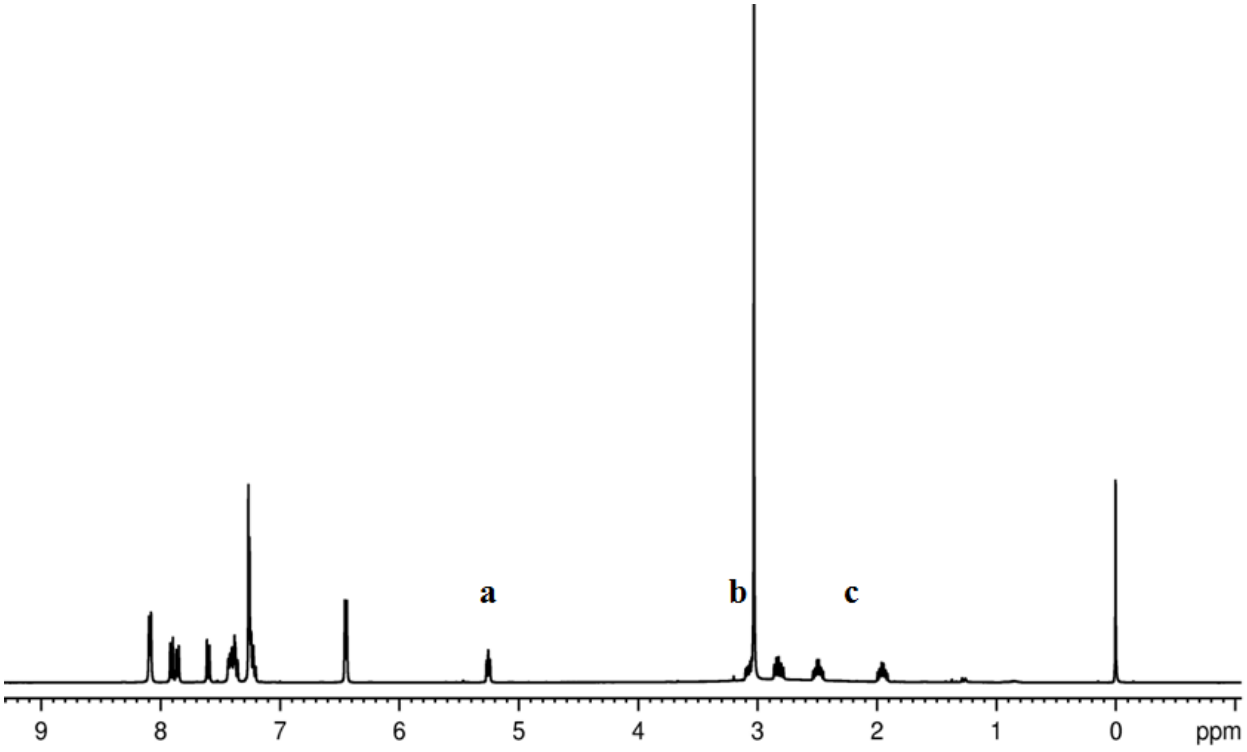


^{1}H-NMR spectrum of (*R/S*)-2-amino-3-methyl-1-butanolin *R*-BNPA and DMAP

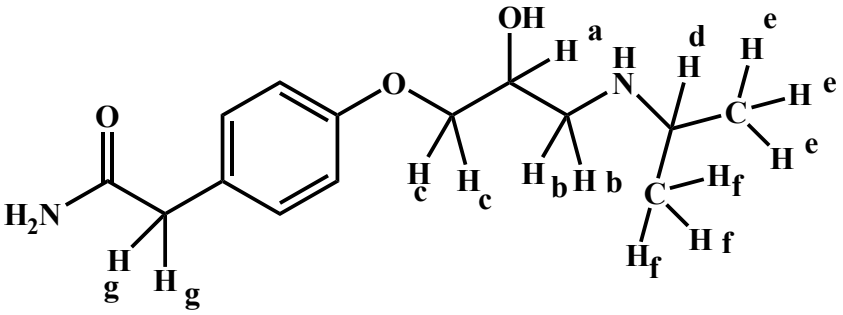


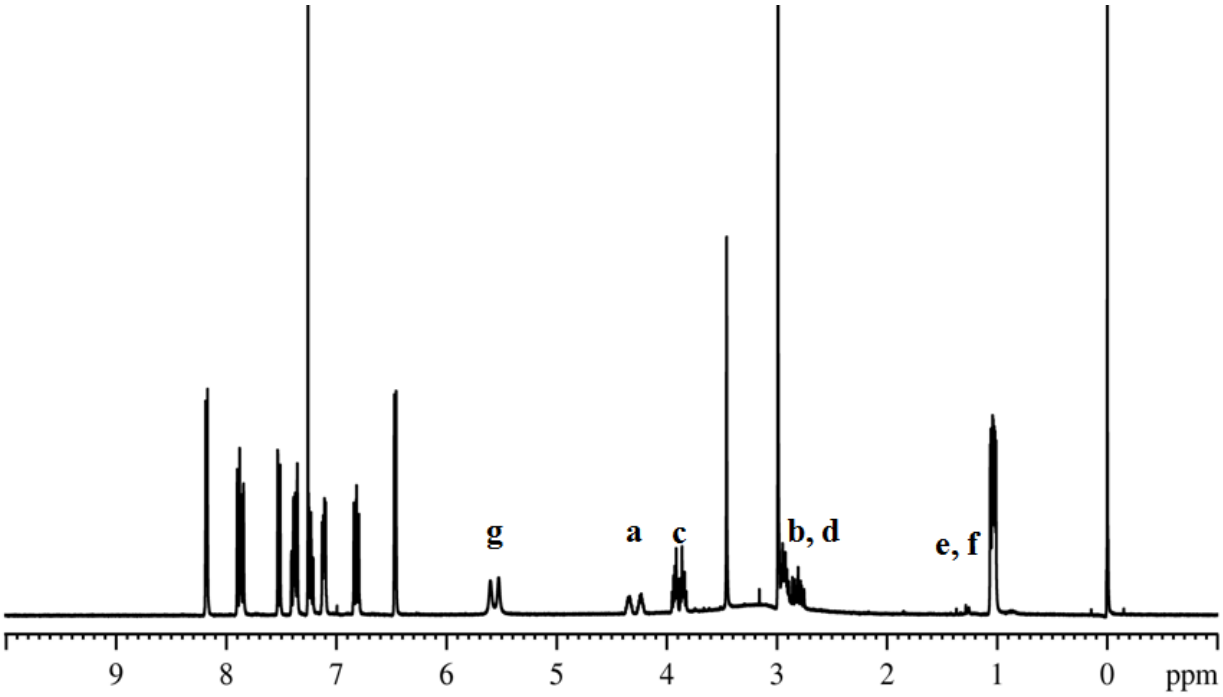
^{1}H-NMR spectrum of (*R/S*)-1-Amino-2-indanolin *R*-BNPA and DMAP



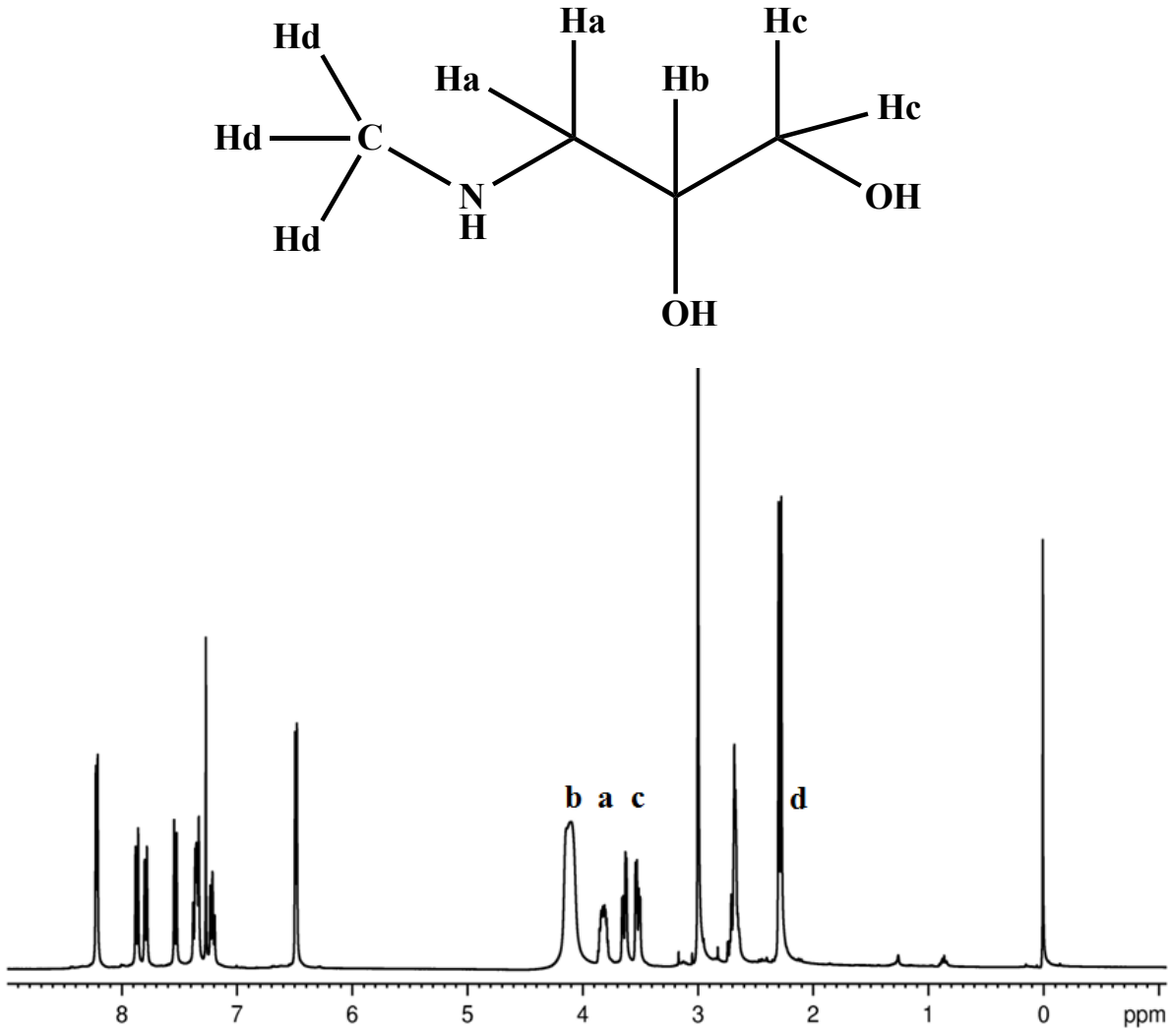


^{1}H-NMR spectrum of (*R/S*)-atenolol in *R*-BNPA and DMAP

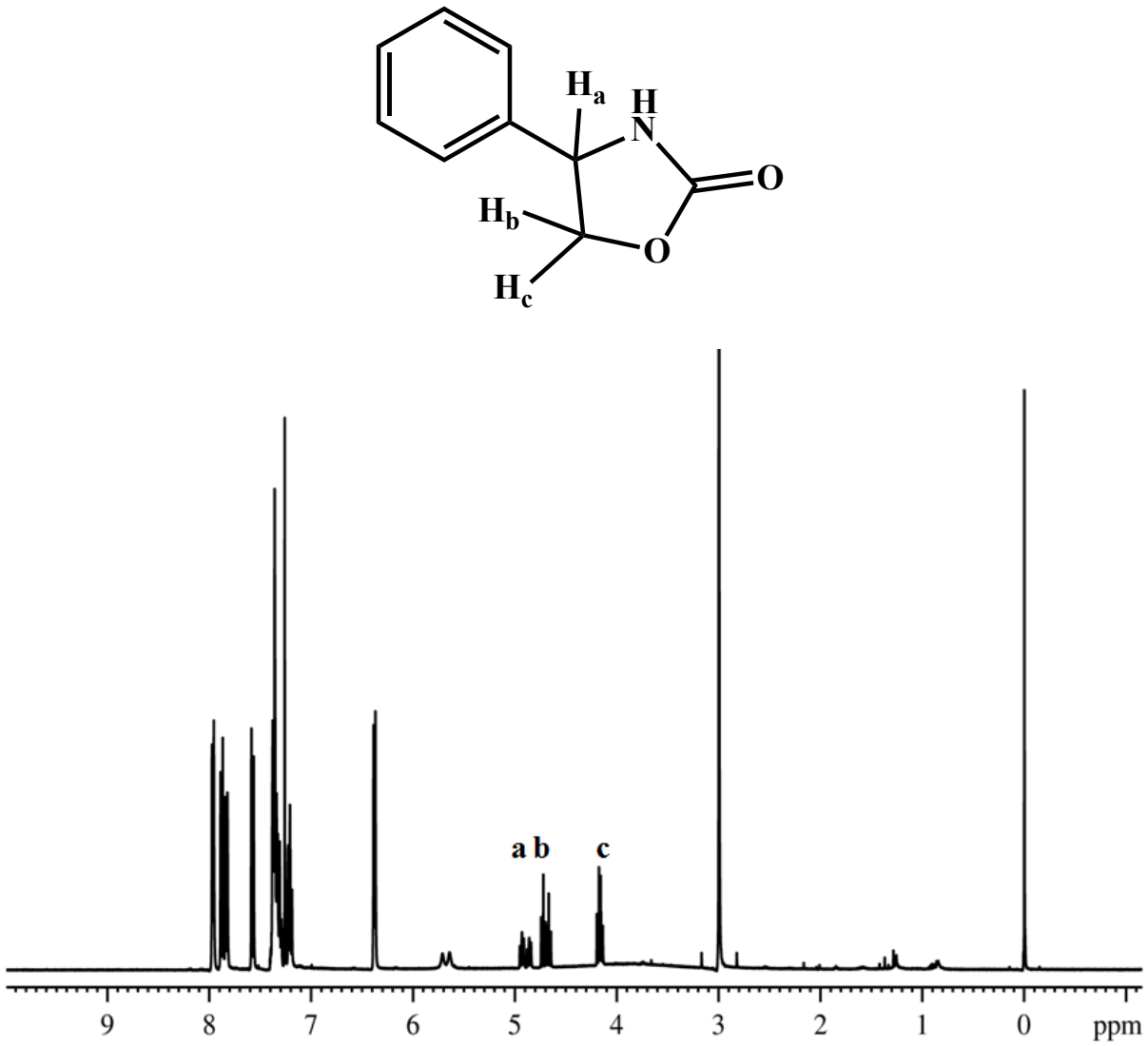




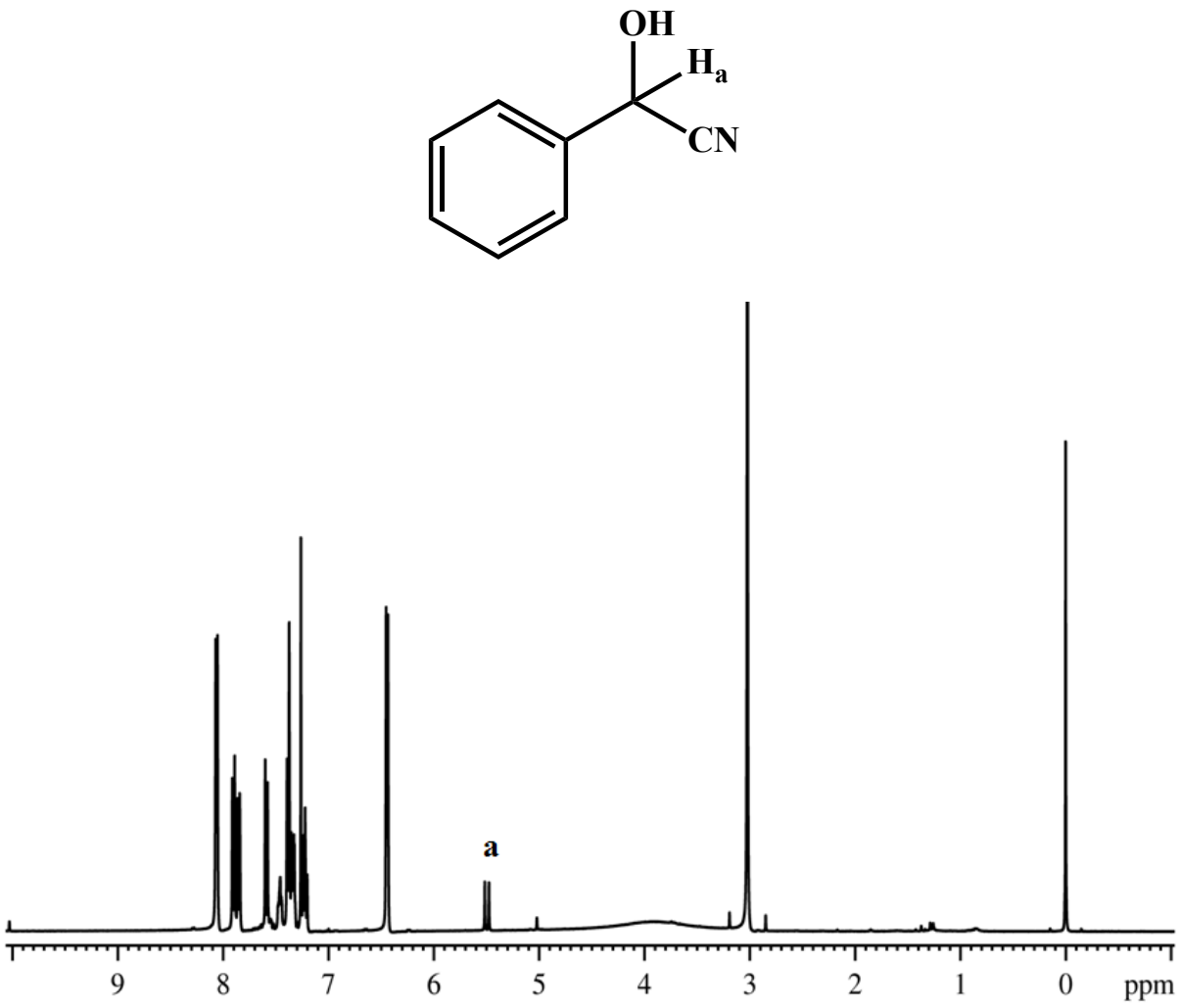
[1]H-NMR spectrum of (*R/S*)-4-phenyl-2-oxazolidinone in *R*-BNPA and DMAP



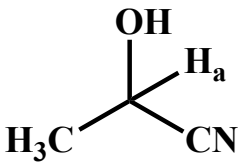
^{1}H-NMR spectrum of (*R/S*)-4-phenyl-2-oxazolidinone in *R*-BNPA and DMAP

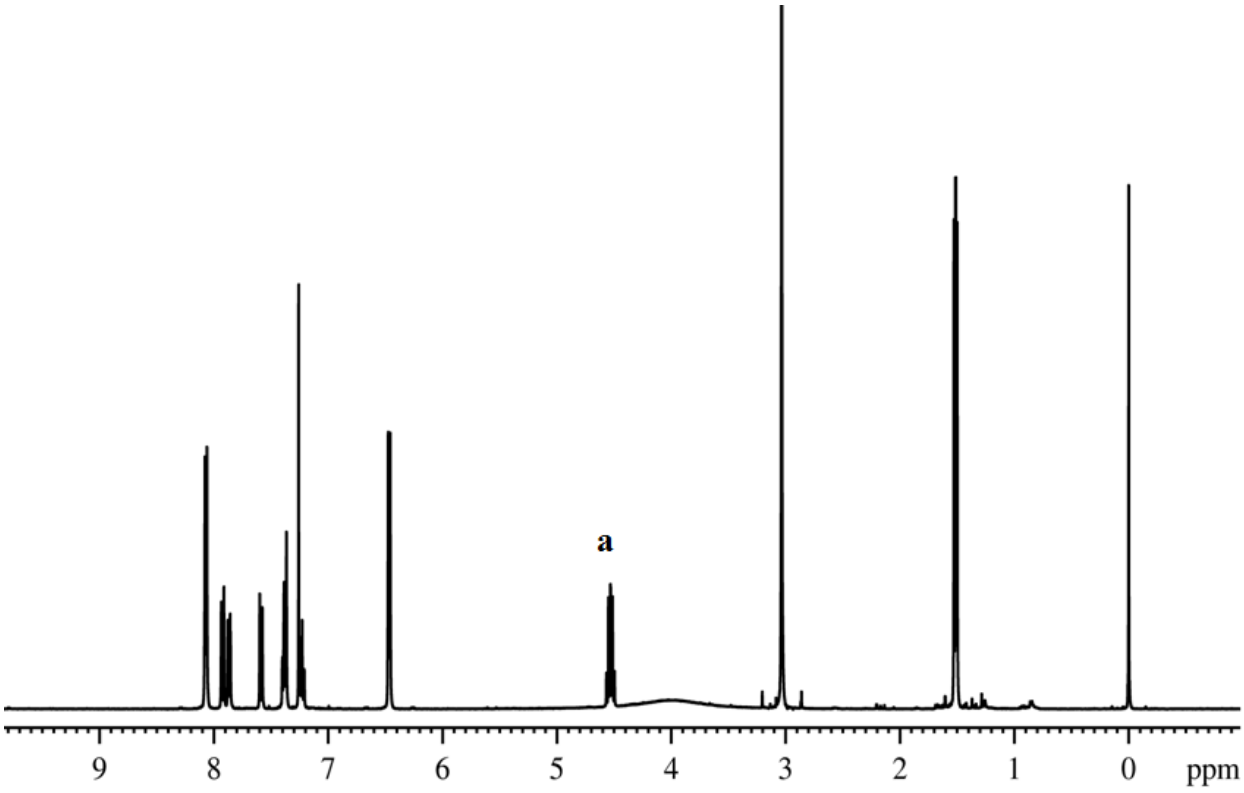


^{1}H-NMR spectrum of (*R/S*)-mandelonitrile in *R*-BNPA and DMAP

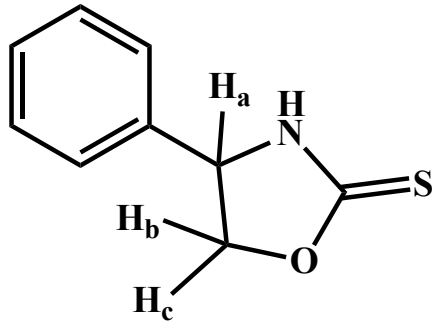


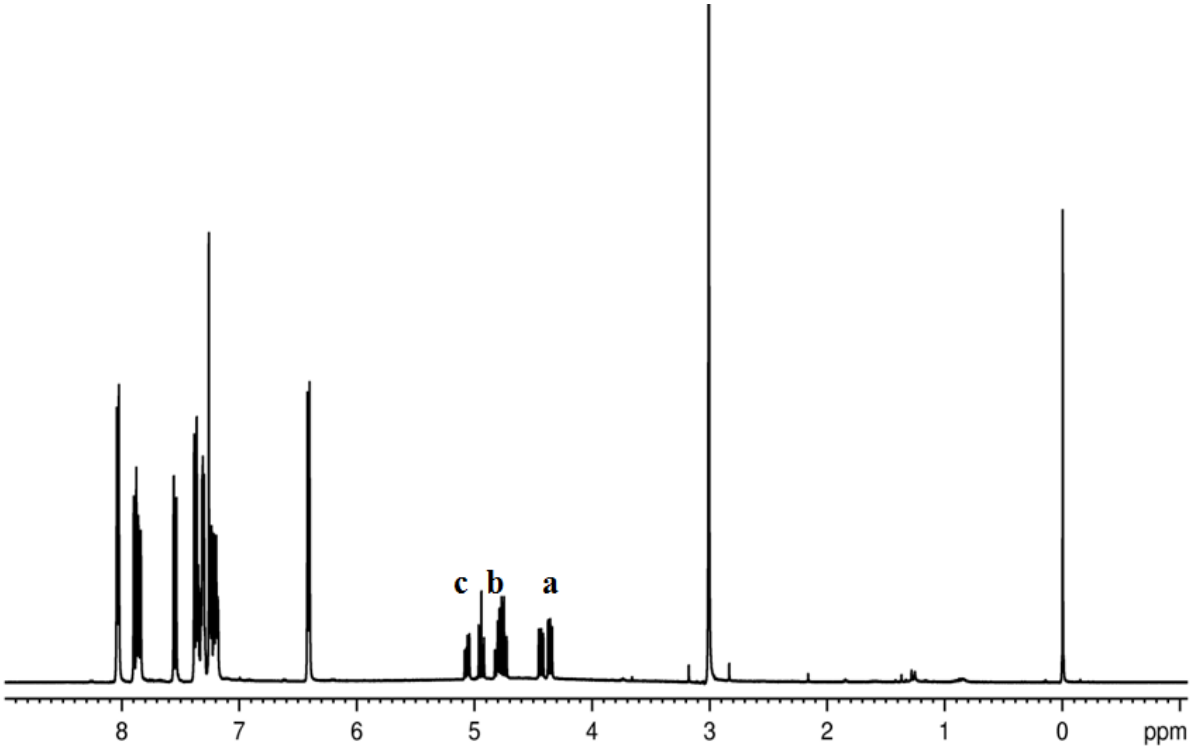
^{1}H-NMR spectrum of (*R/S*)-lactonitrile in *R*-BNPA and DMAP



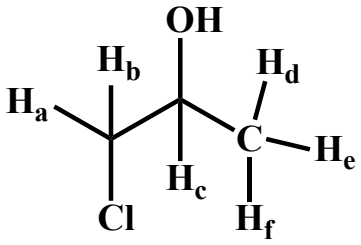


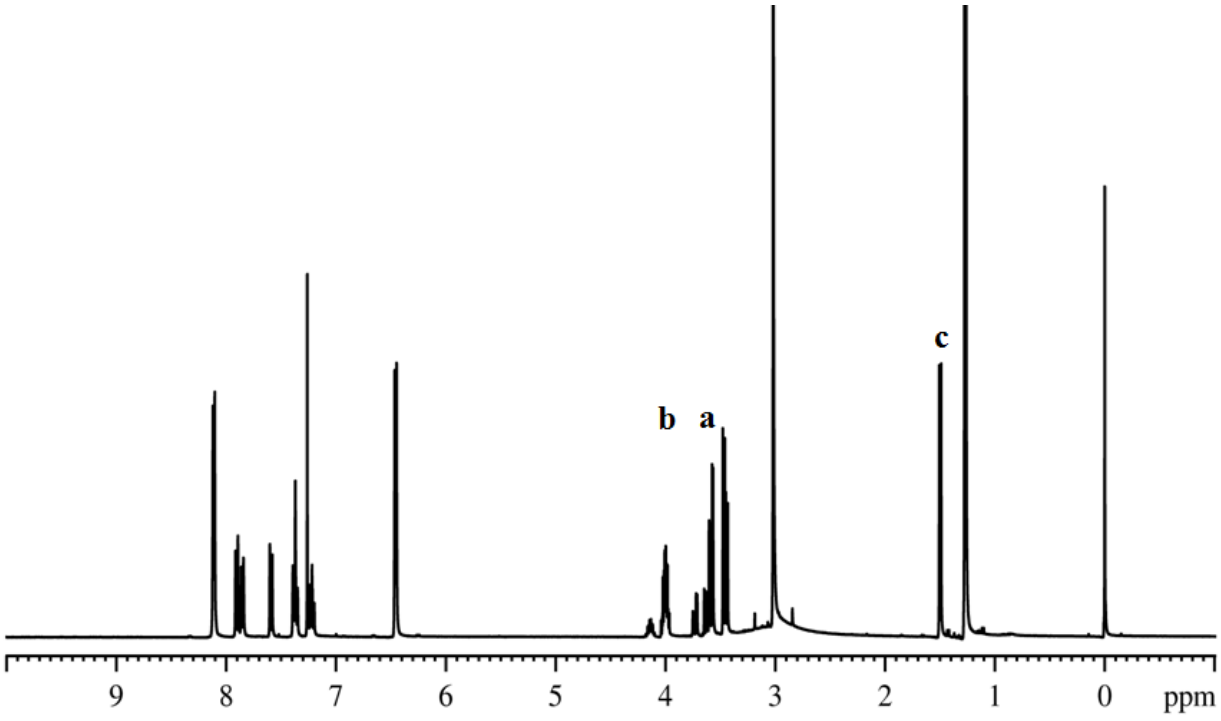
^{1}H-NMR spectrum of (*R/S*)-4-phenyl oxazolidine-2-thione in *R*-BNPA and DMAP



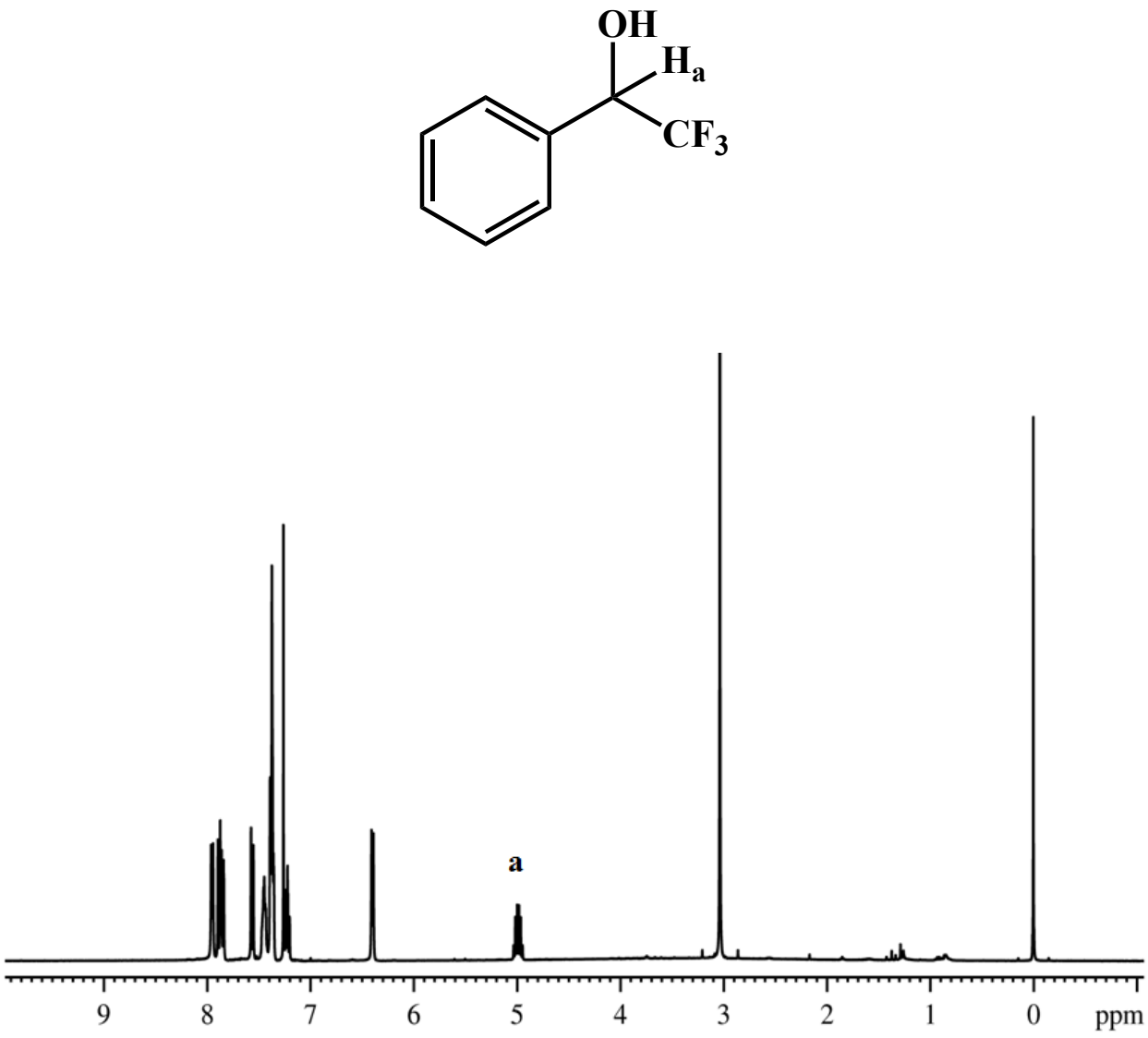


[1]H-NMR spectrum of (*R/S*)-1-chloro-2-propanol in *R*-BNPA and DMAP

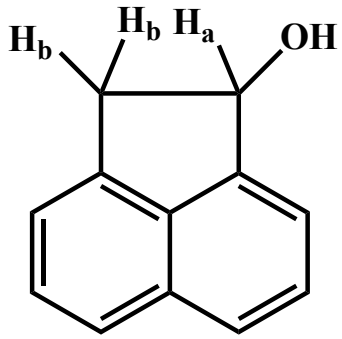


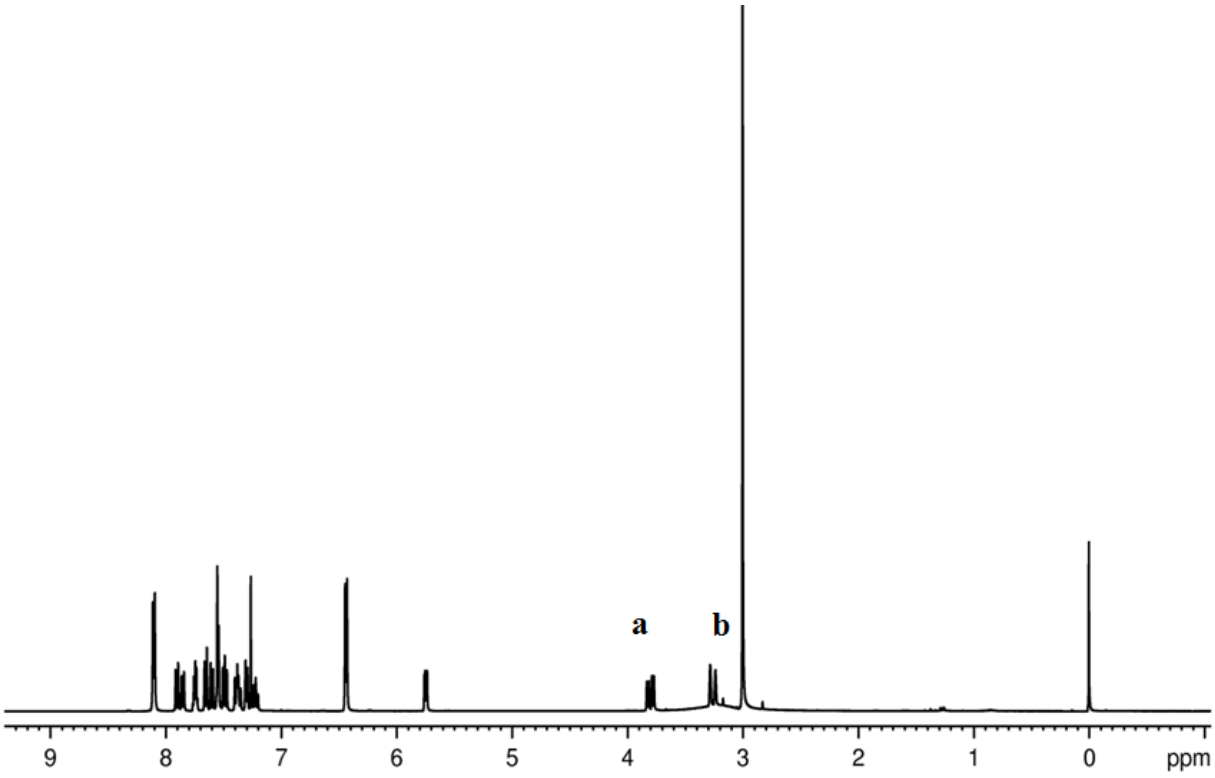


^{1}H-NMR spectrum of (*R/S*)-α-trifluoromethyl benzyl alcohol in *R*-BNPA and DMAP

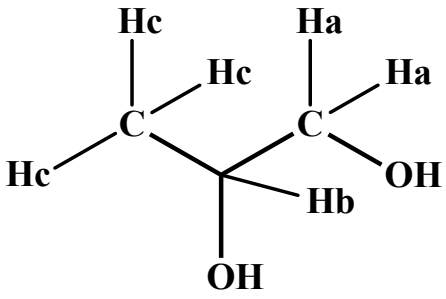


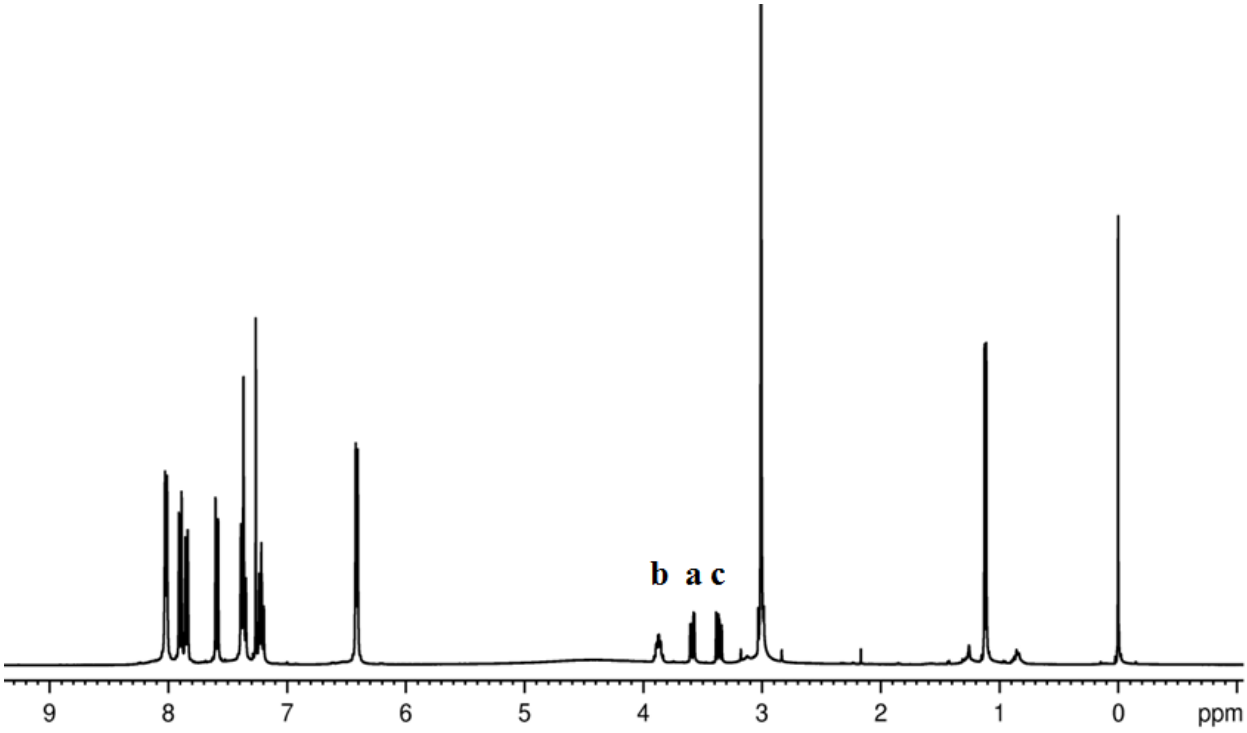
^{1}H-NMR spectrum of (*R/S*)-1-acenapthenol benzyl alcohol in *R*-BNPA and DMAP



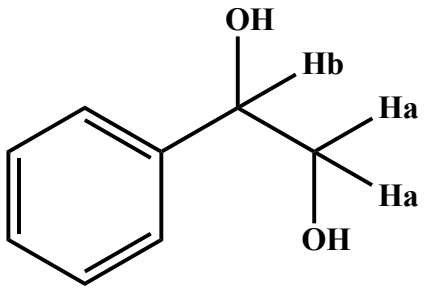


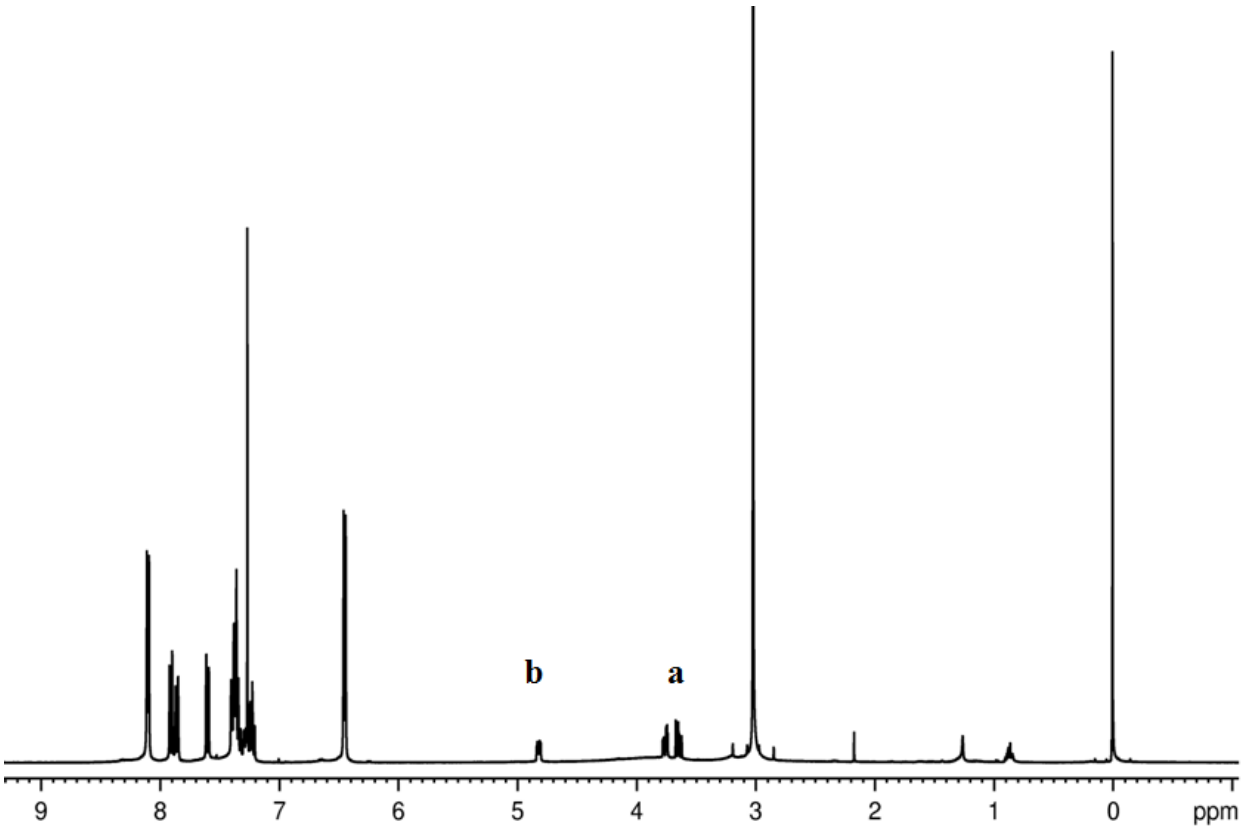
^{1}H-NMR spectrum of (*R/S*)-1, 2-propanediol in *R*-BNPA and DMAP



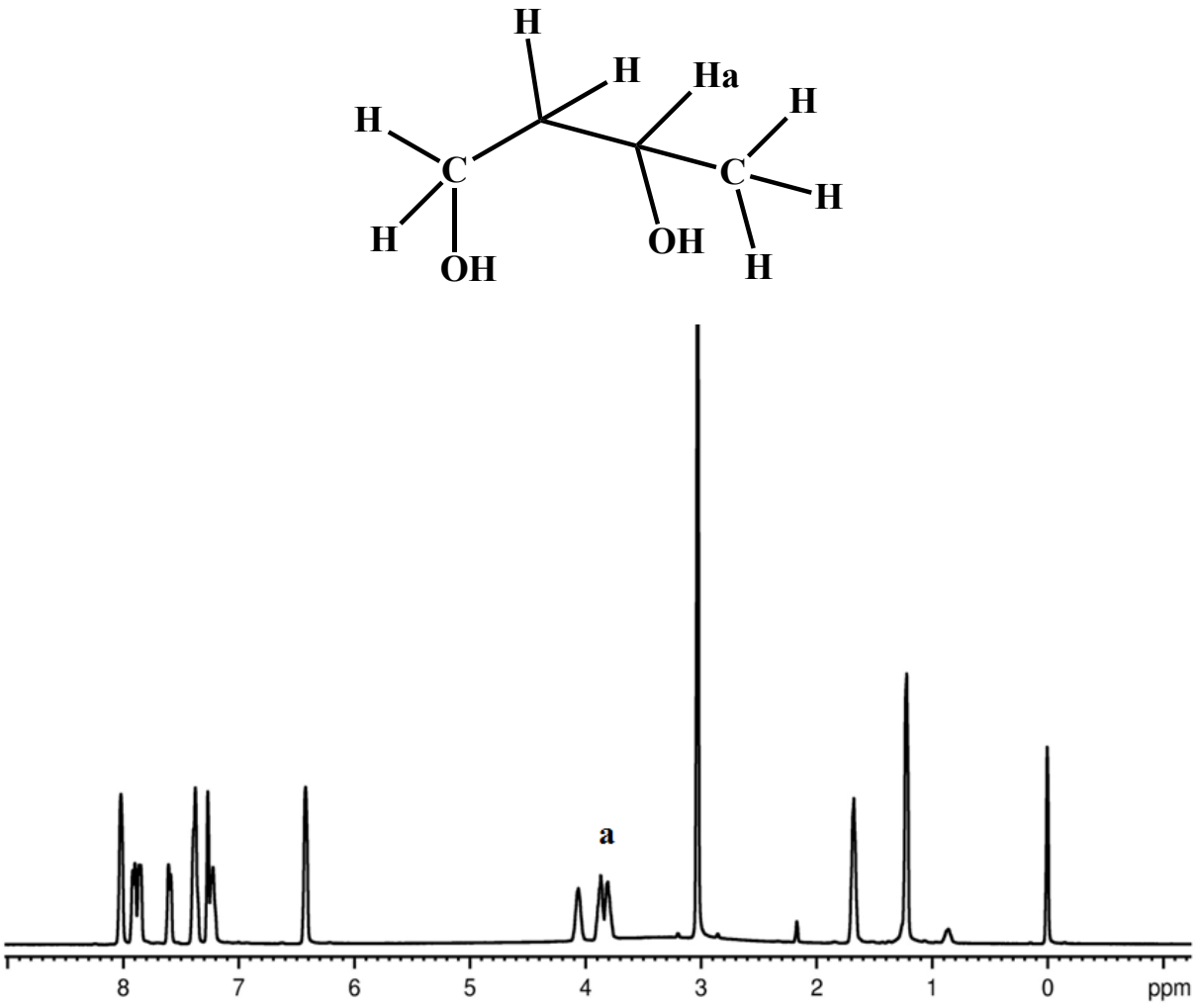


^{1}H-NMR spectrum of (*R/S*)-1,2-propanediol in *R*-BNPA and DMAP

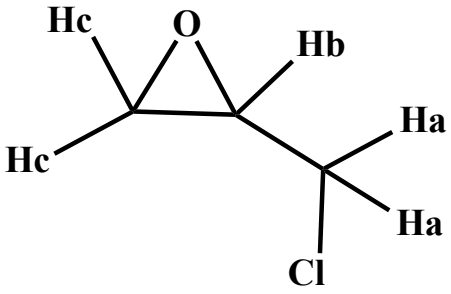


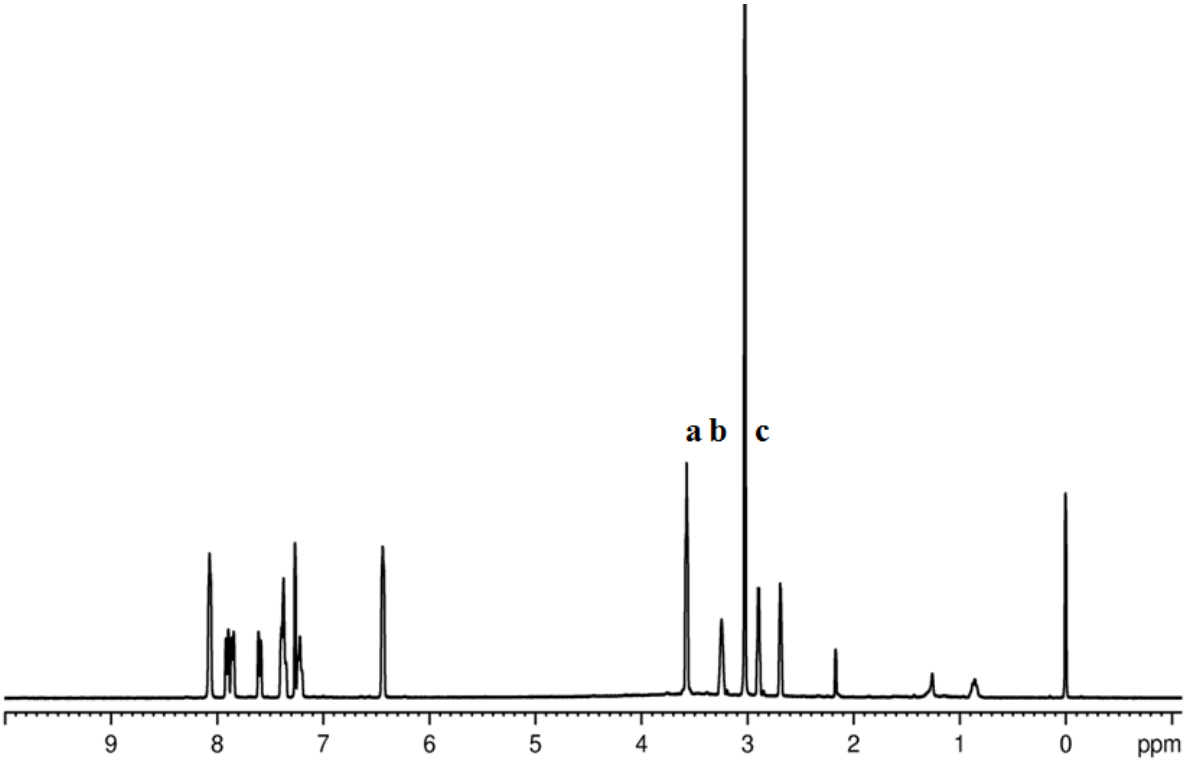


[1]H-NMR spectrum of (*R/S*)-1,3-butanediol in *R*-BNPA and DMAP

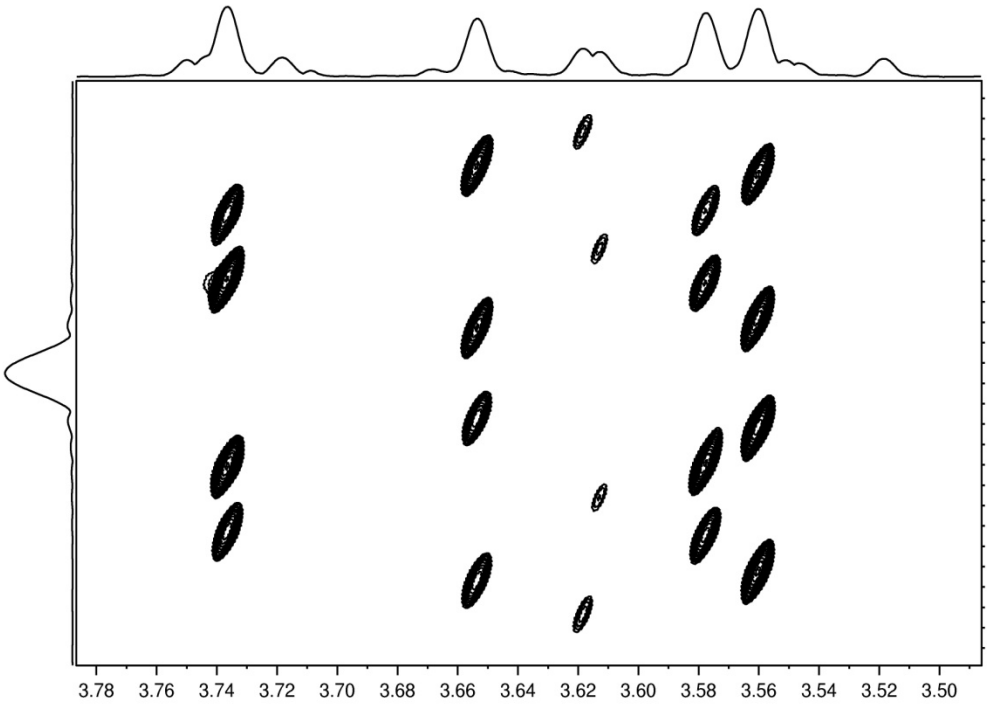


[1]H-NMR spectrum of (*R/S*)-epichlorohydrinin *R*-BNPA and DMAP

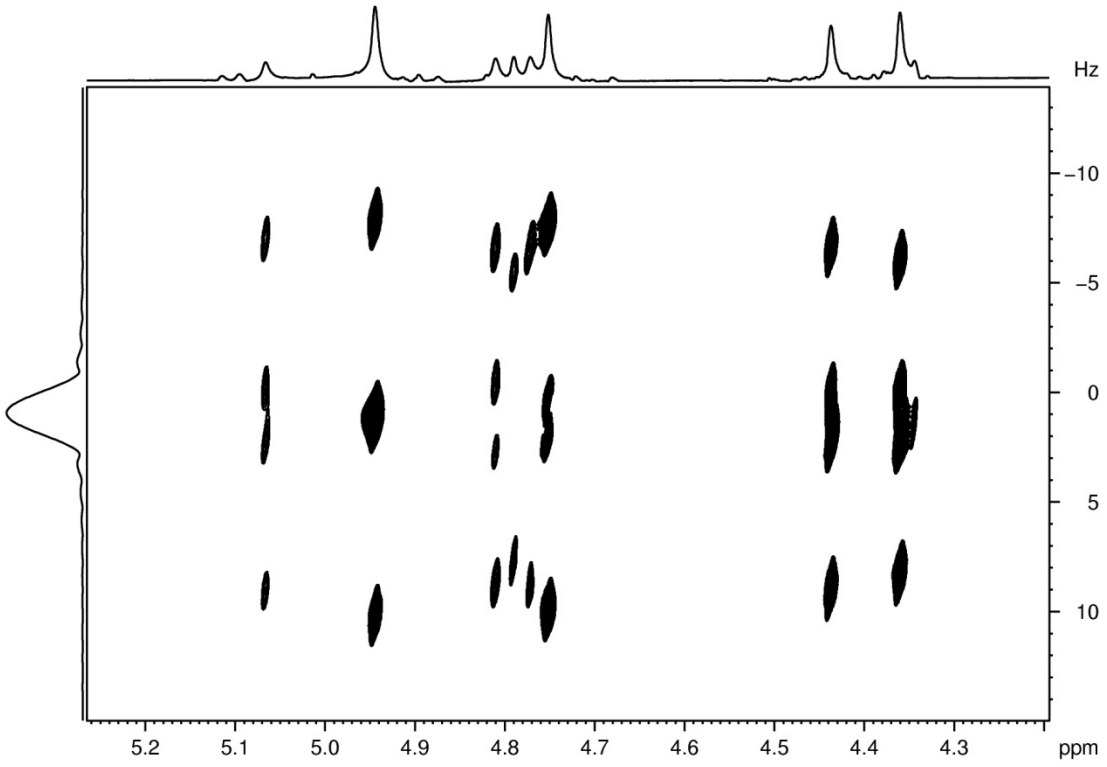




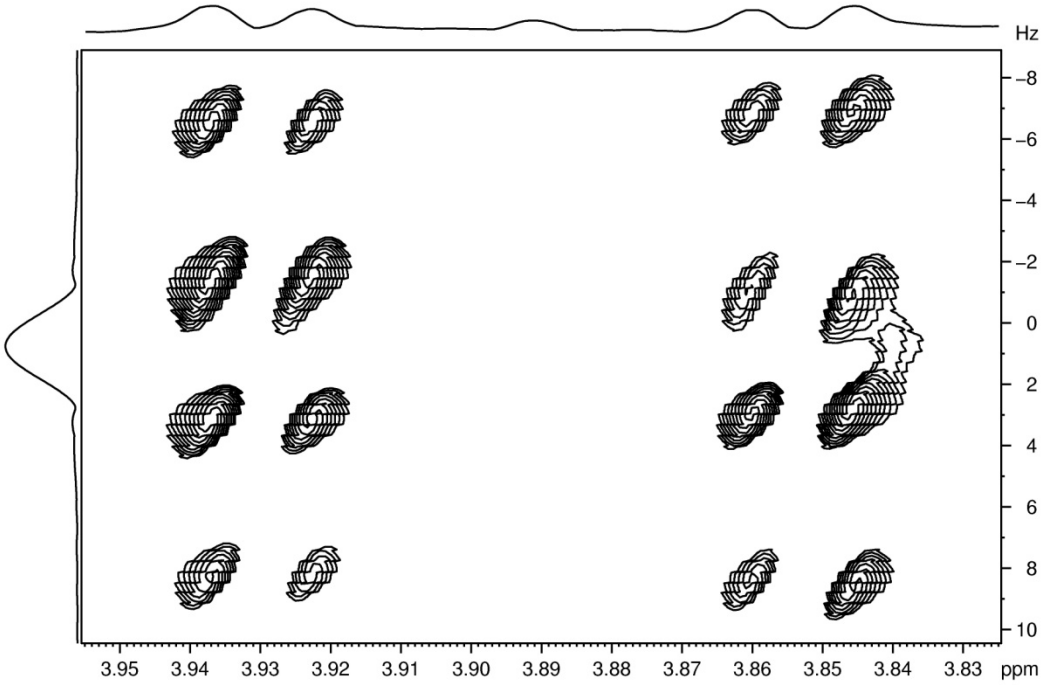
45^0 skew projected 2D *J*-resolved spectra of (*R/S*)-2-piperidinemethanol in *R*-BNPA and DMAP



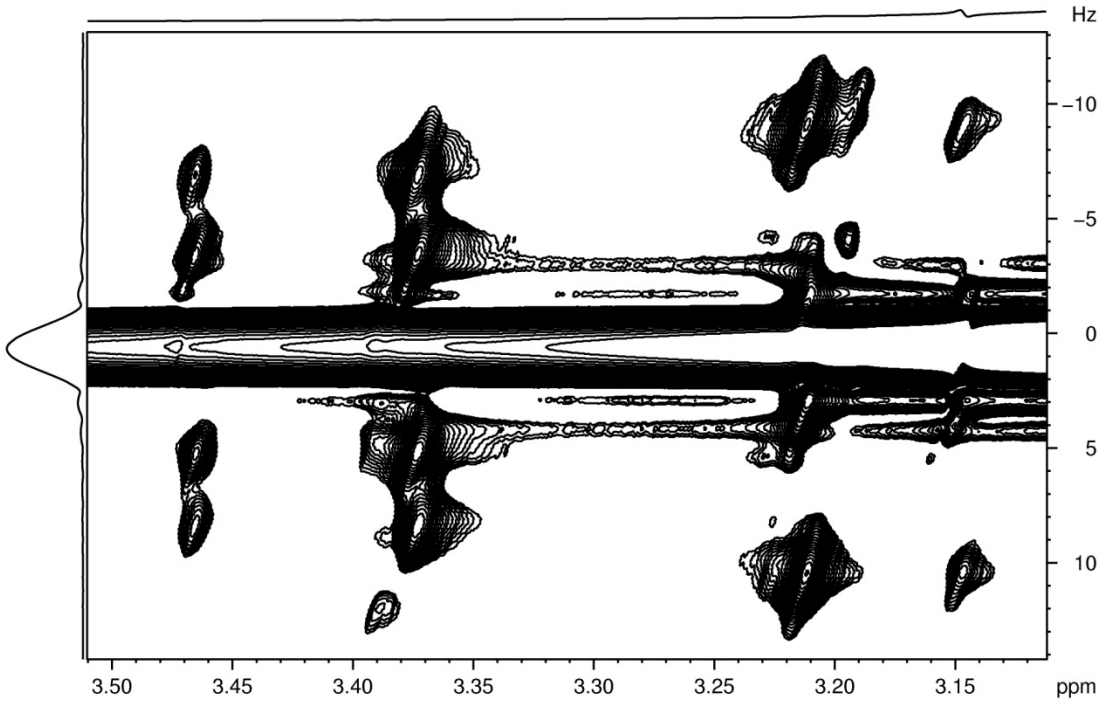
45^0 skew projected 2D *J*-resolved spectra of (*R/S*)-2-amino-2-phenylethanol in *R*-BNPA and DMAP



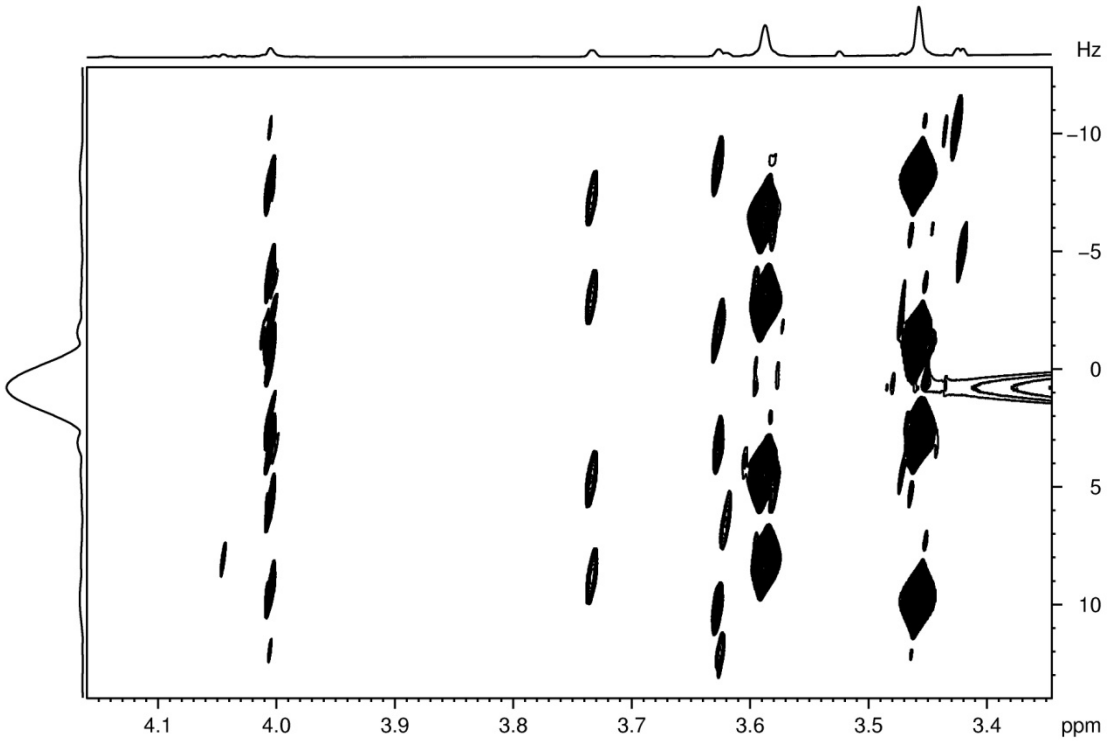
45^0 skew projected 2D J-resolved spectra of (*R/S*)-atenolol in *R*-BNPA and DMAP



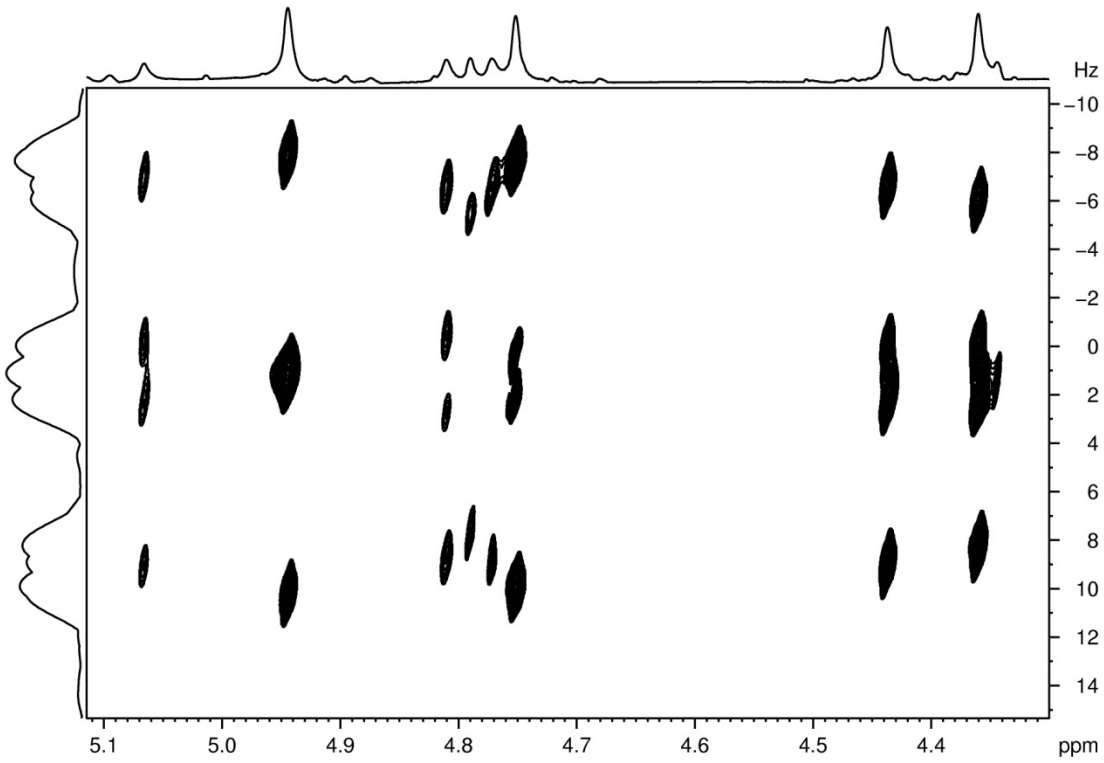
45^0 skew projected 2D J-resolved spectra of (*R/S*)-2-aminobutanol in *R*-BNPA and DMAP



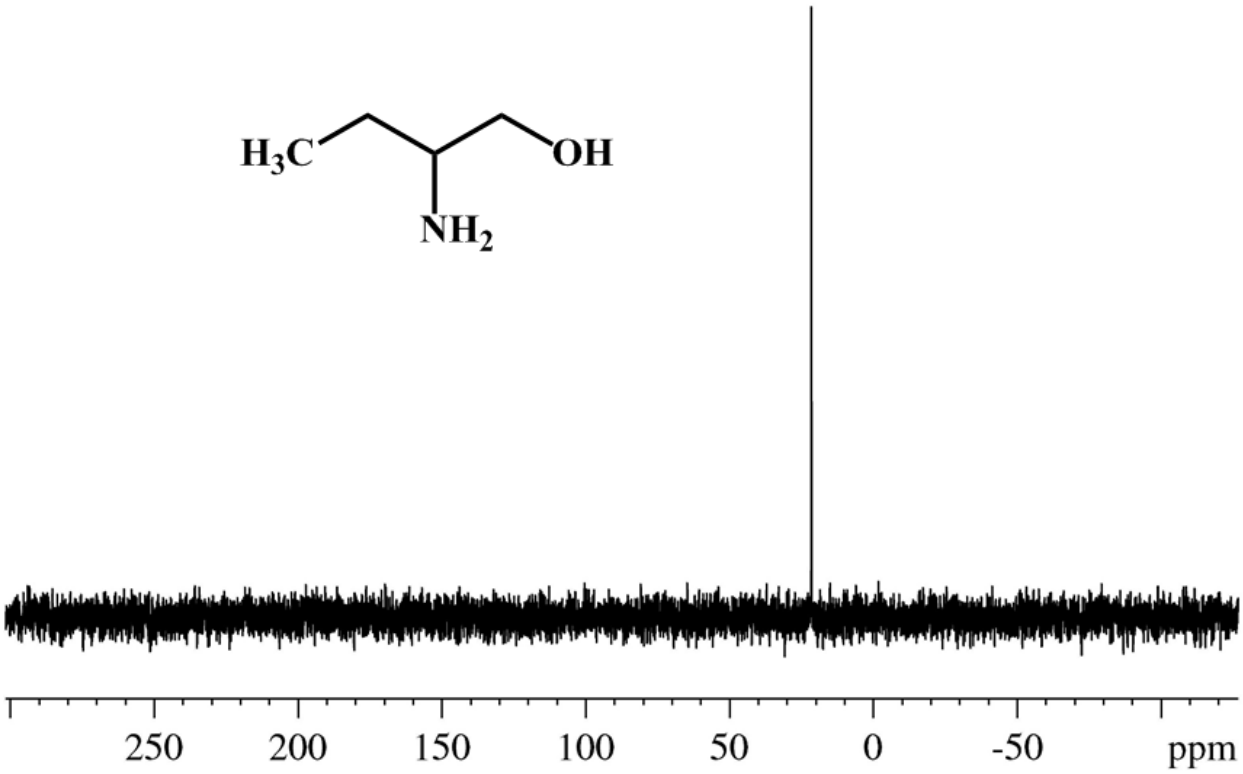
45^0 skew projected 2D J-resolved spectra of (*R/S*)- 1-chloro-2-propanolnol in *R*-BNPA and DMAP



45^0 skew projected 2D J-resolved spectrum of (*R/S*)-4-phenyl oxazolidine-2-thione in *R*-BNPA and DMAP



^{31}P-NMR spectrum of racemic 2-aminobtanol in *R*-BNPA and DMAP



(a) ^{31}P-NMR spectrum of *R*-2-aminobtanol in *R*-BNPA and DMAP and (b) ^{31}P-NMR spectrum of *S*-2-aminobtanol in in *R*-BNPA and DMAP