Electronic Supplementary Material (ESI) for ChemComm.

SUPPORTING INFORMATION

Enantio-differentiation of Molecules with Diverse Functionalities by a Single Probe

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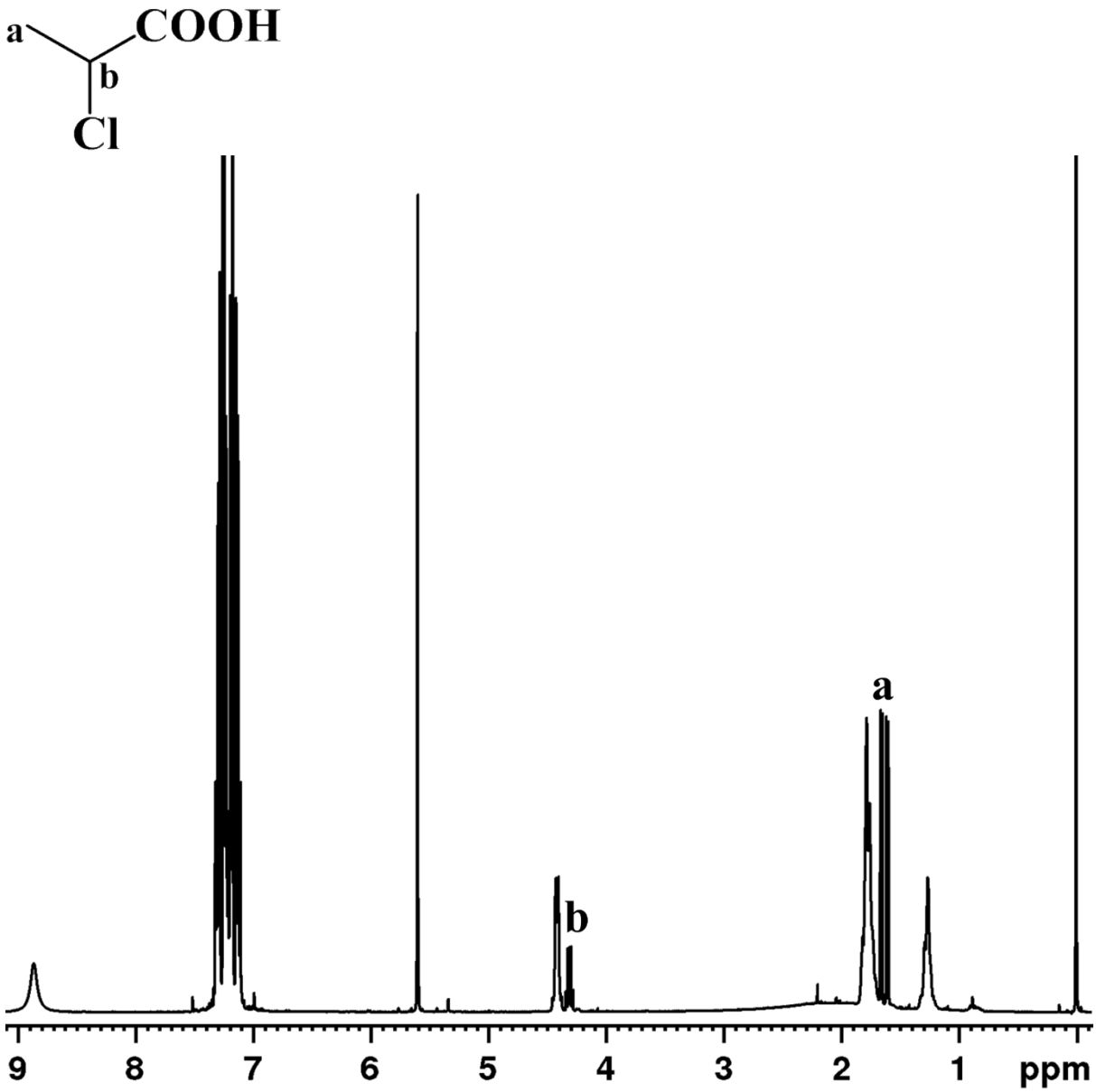
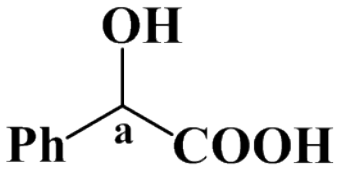
Experimental section

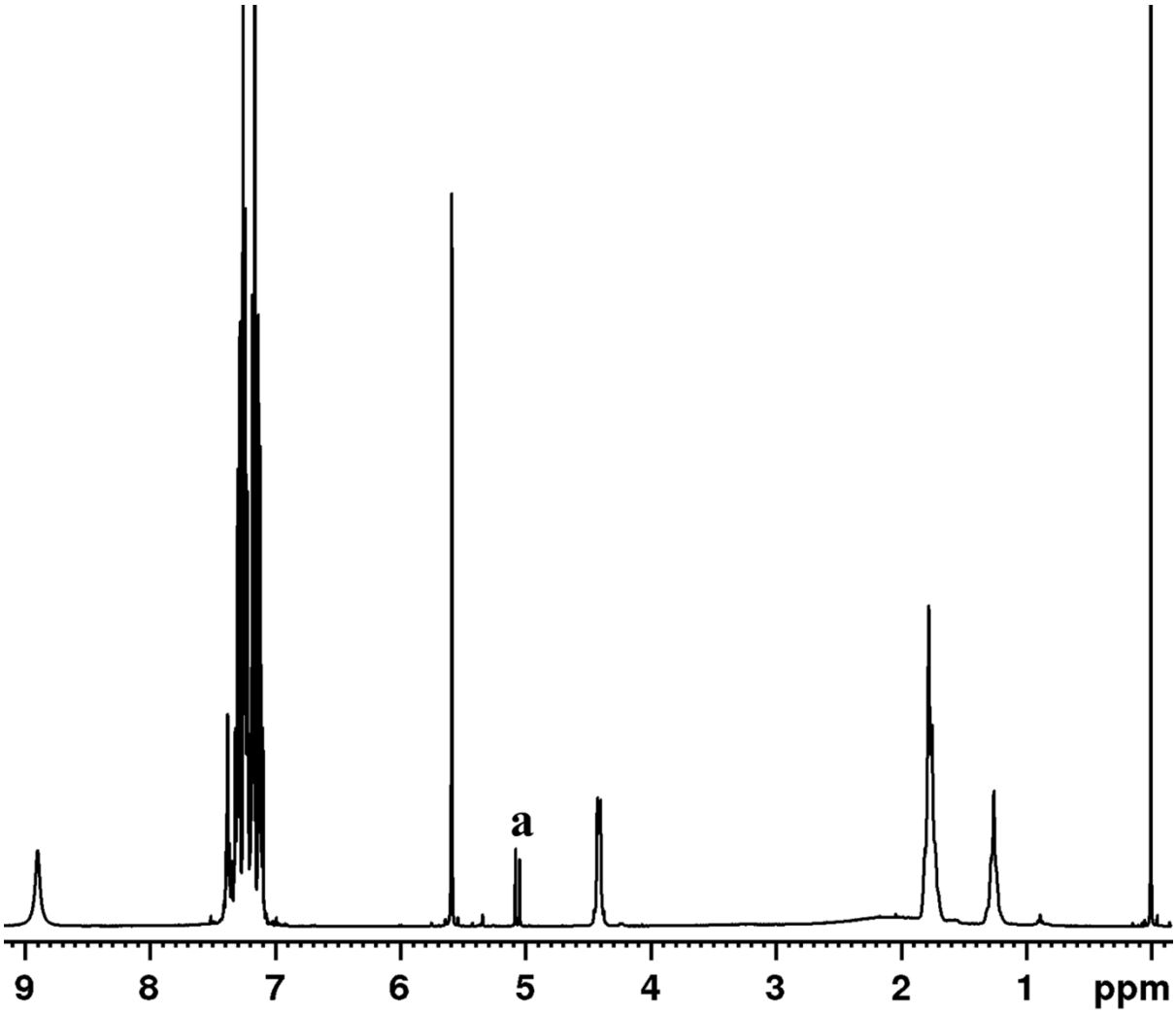
The commercially available (1*S*,2*S*) -N,N'-Dihydroxy-N,N'-bis (diphenylacetyl)-1,2-cyclohexanediamine ((*S*)-CBHA-DPA), the molecules **1-24**, and chloroform-d were purchased and used as received. The ^{1}H and ^{13}C NMR spectra were recorded on 400MHz spectrometer and referenced with respect to TMS. The pure shift NMR spectra were recorded on 500 MHz spectrometer.

400MHz ^{1}H-NMR spectrum of (*R/S*)-2-chloropropanoic acid and (*S*)-CBHA-DPA in $CDCl_3$

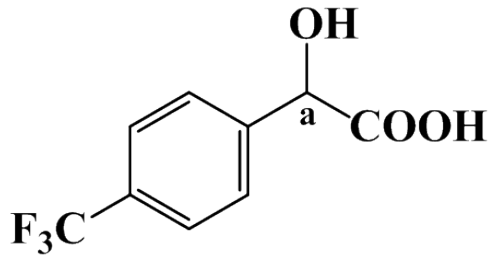


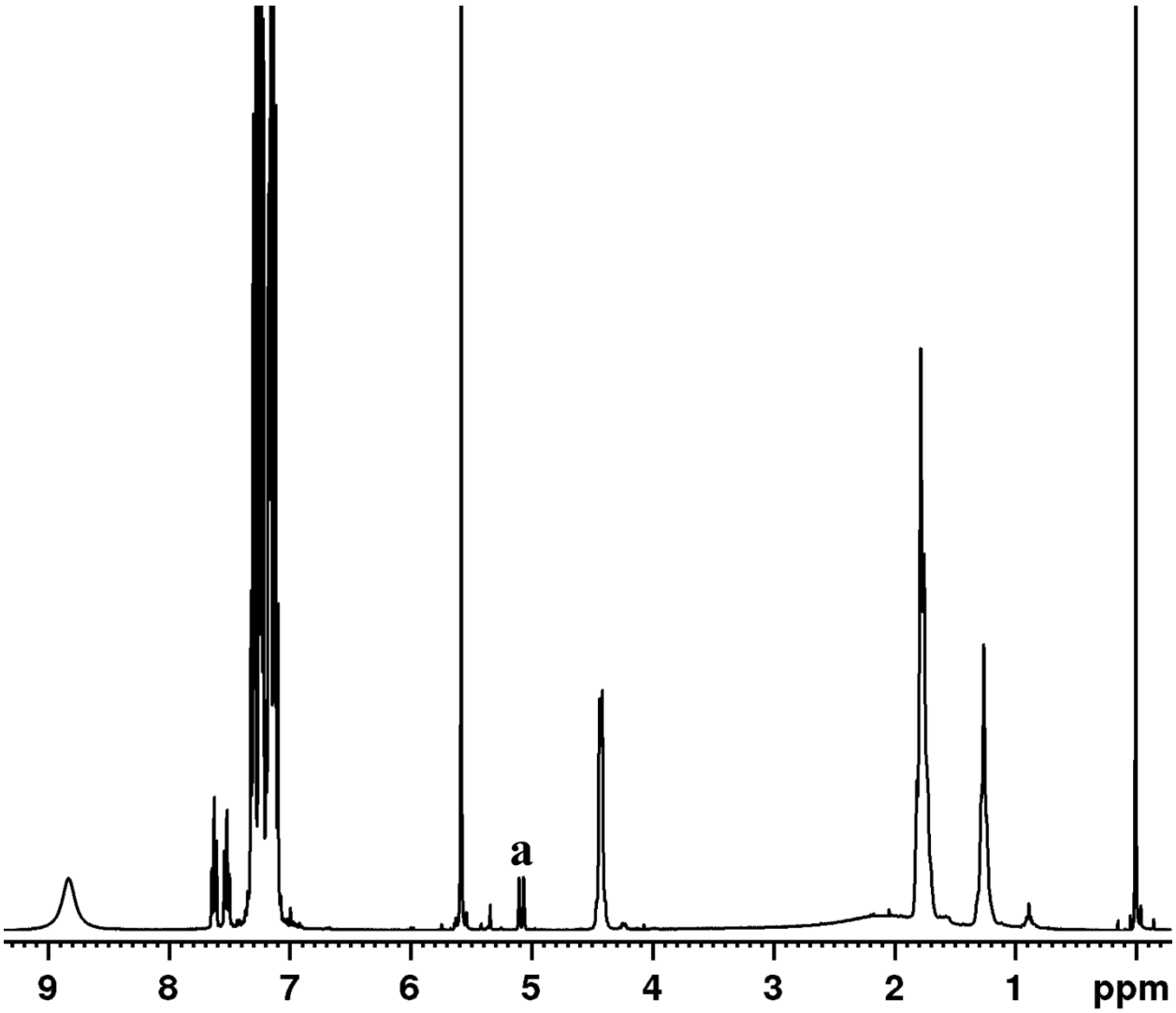
400MHz ^{1}H-NMR spectrum of (*R/S*) - Mandelic acid and (*S*)-CBHA-DPA in $CDCl_3$



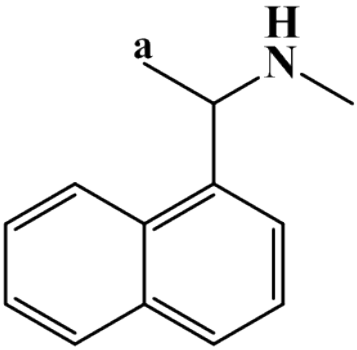


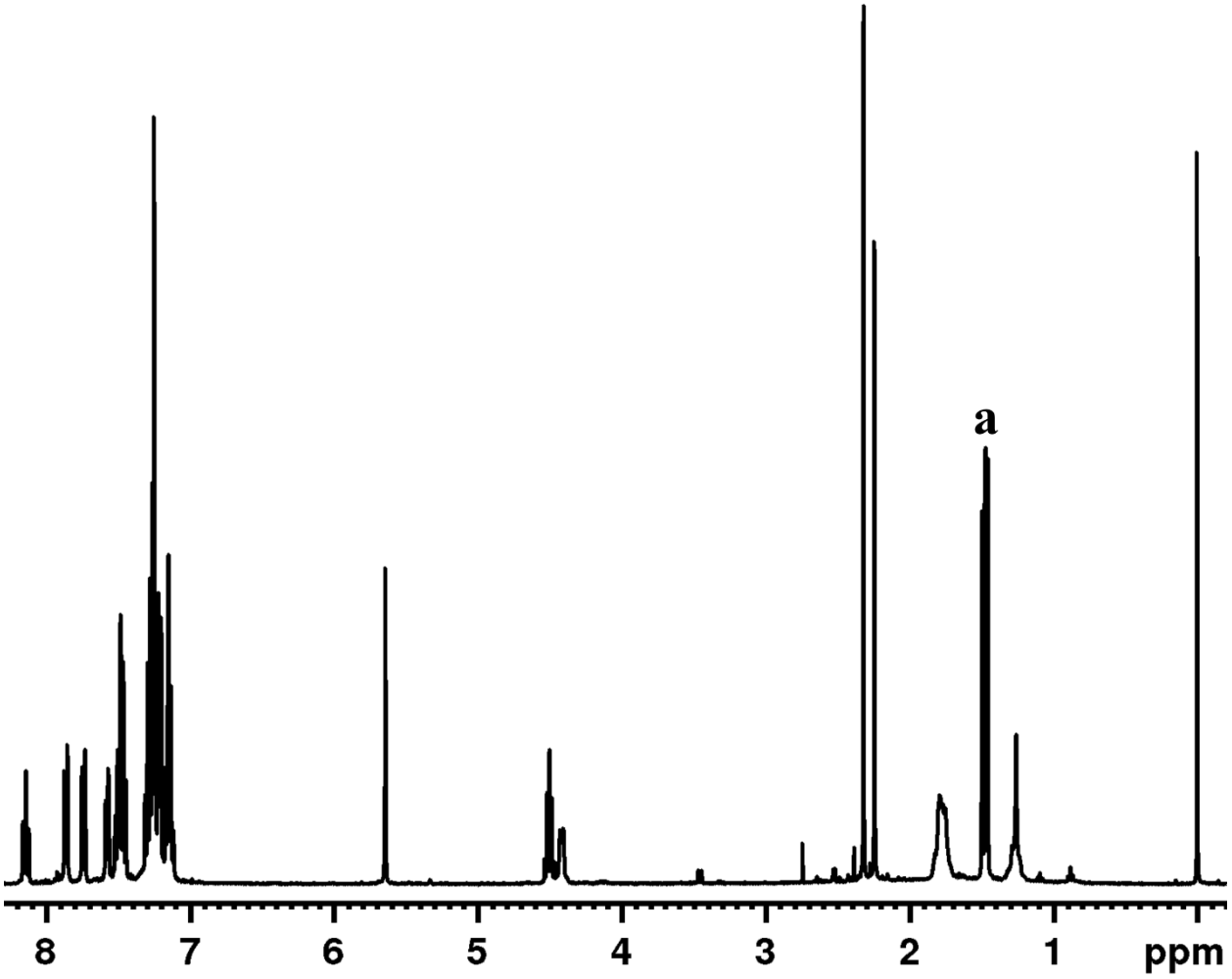
400MHz ^{1}H-NMR spectrum of (*R/S*) - 4-(Trifluoromethyl) mandelic acid and (*S*)-CBHA-DPA in $CDCl_3$



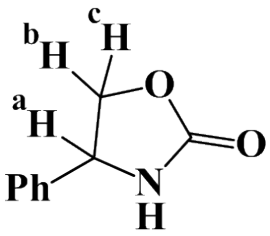


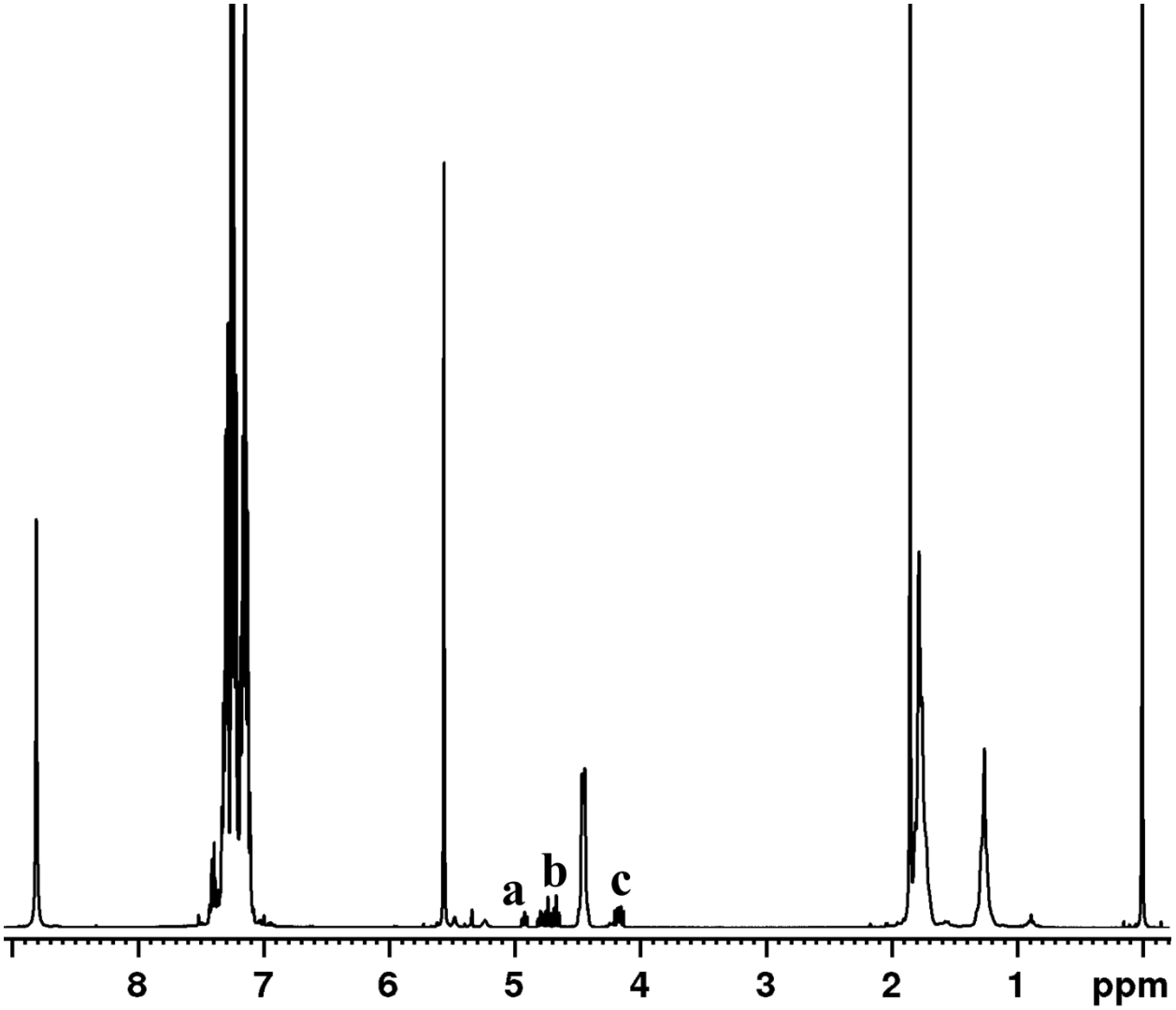
400MHz ^{1}H-NMR spectrum of (*R/S*) - N-Methyl-1-(1-naphthyl)ethylamineand(*S*)-CBHA-DPA in $CDCl_3$



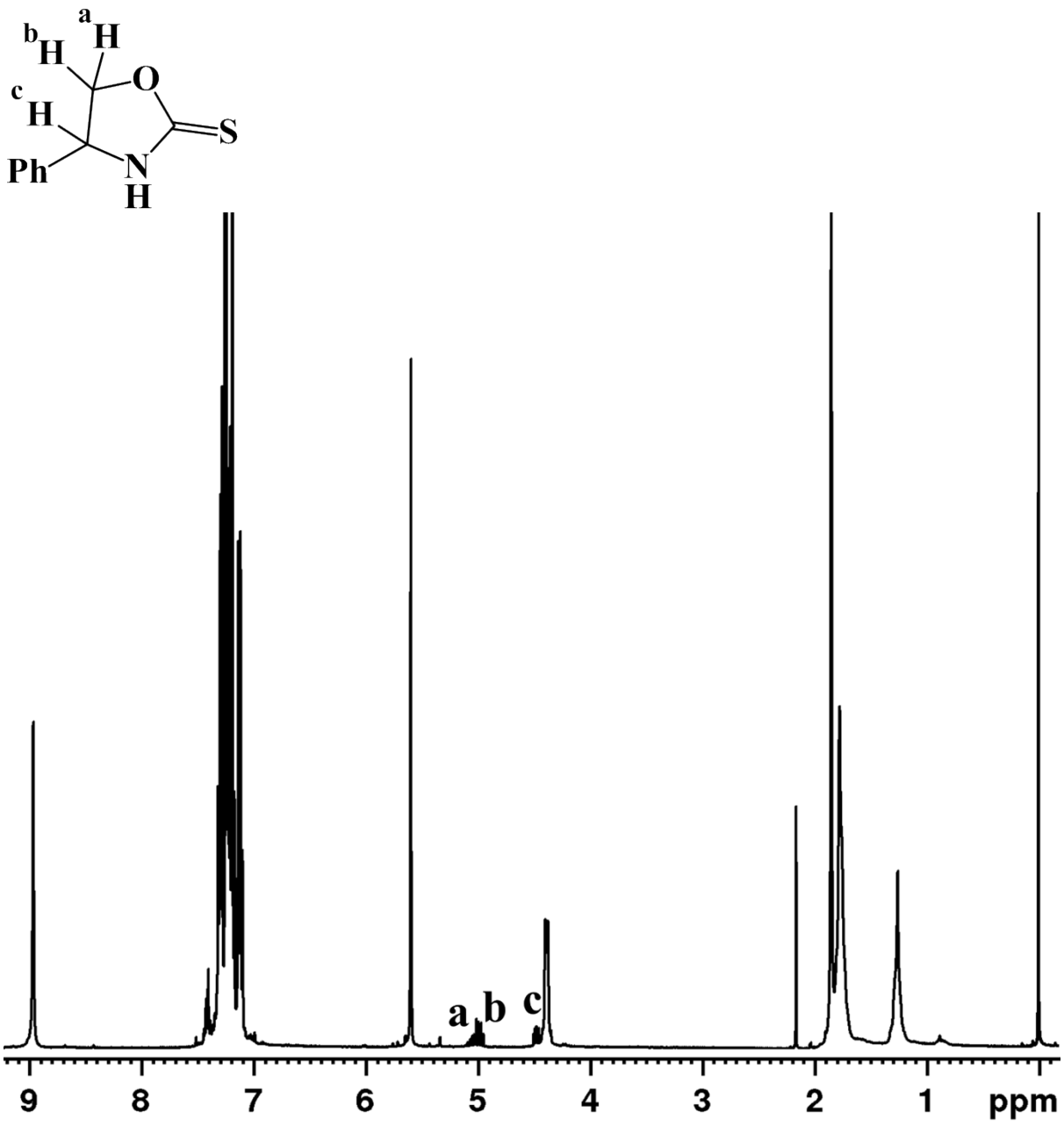


400MHz ^{1}H-NMR spectrum of (*R/S*)-4-phenyloxazolidin-2-one and (*S*)-CBHA-DPA in $CDCl_3$

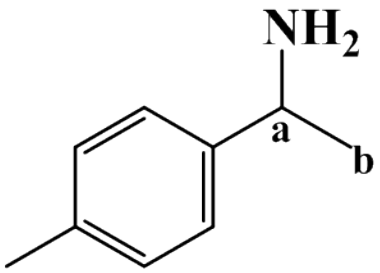


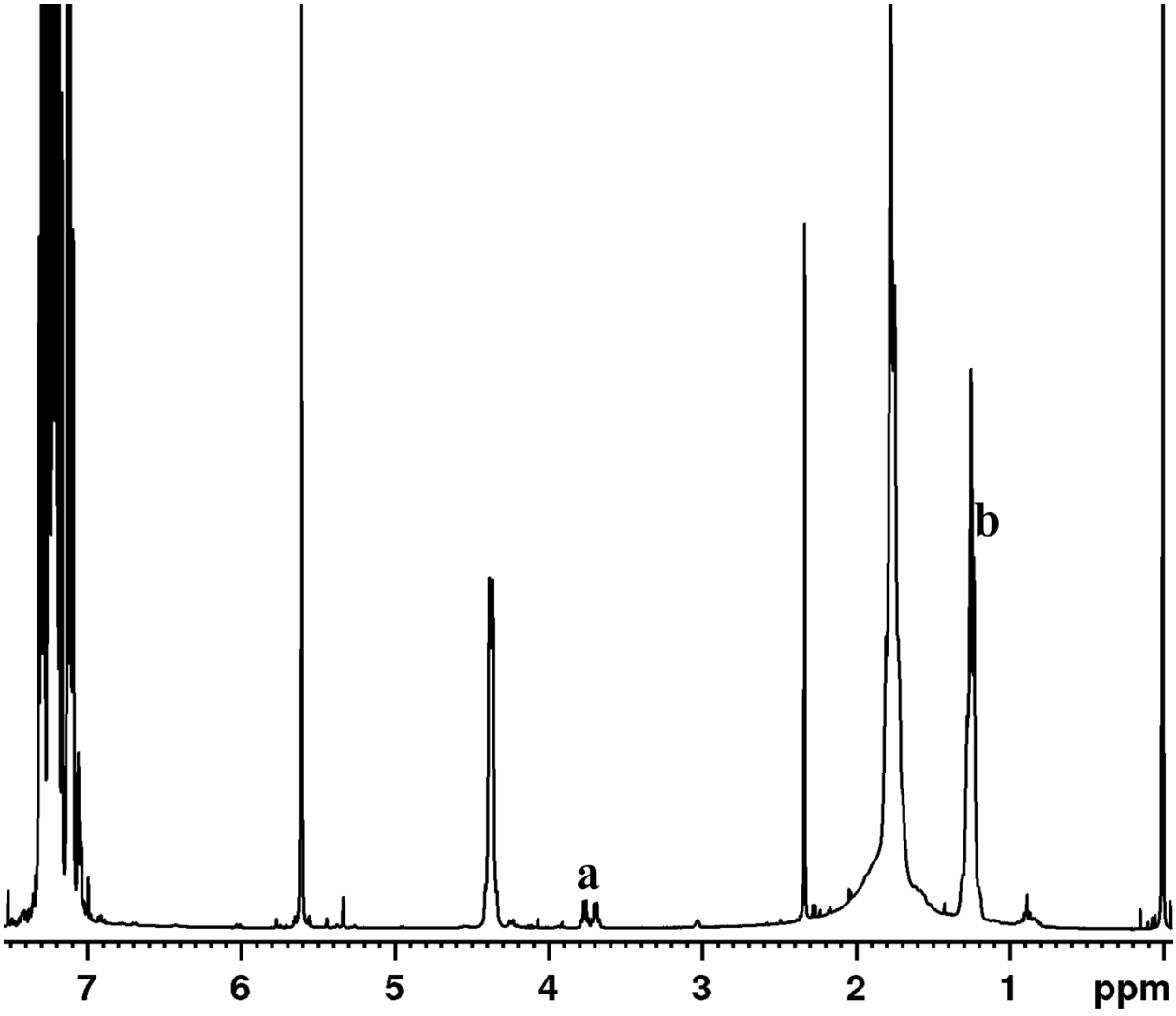


400MHz ^{1}H-NMR spectrum of (*R/S*)-4-phenyloxazolidine-2-thione and (*S*)-CBHA-DPA in $CDCl_3$

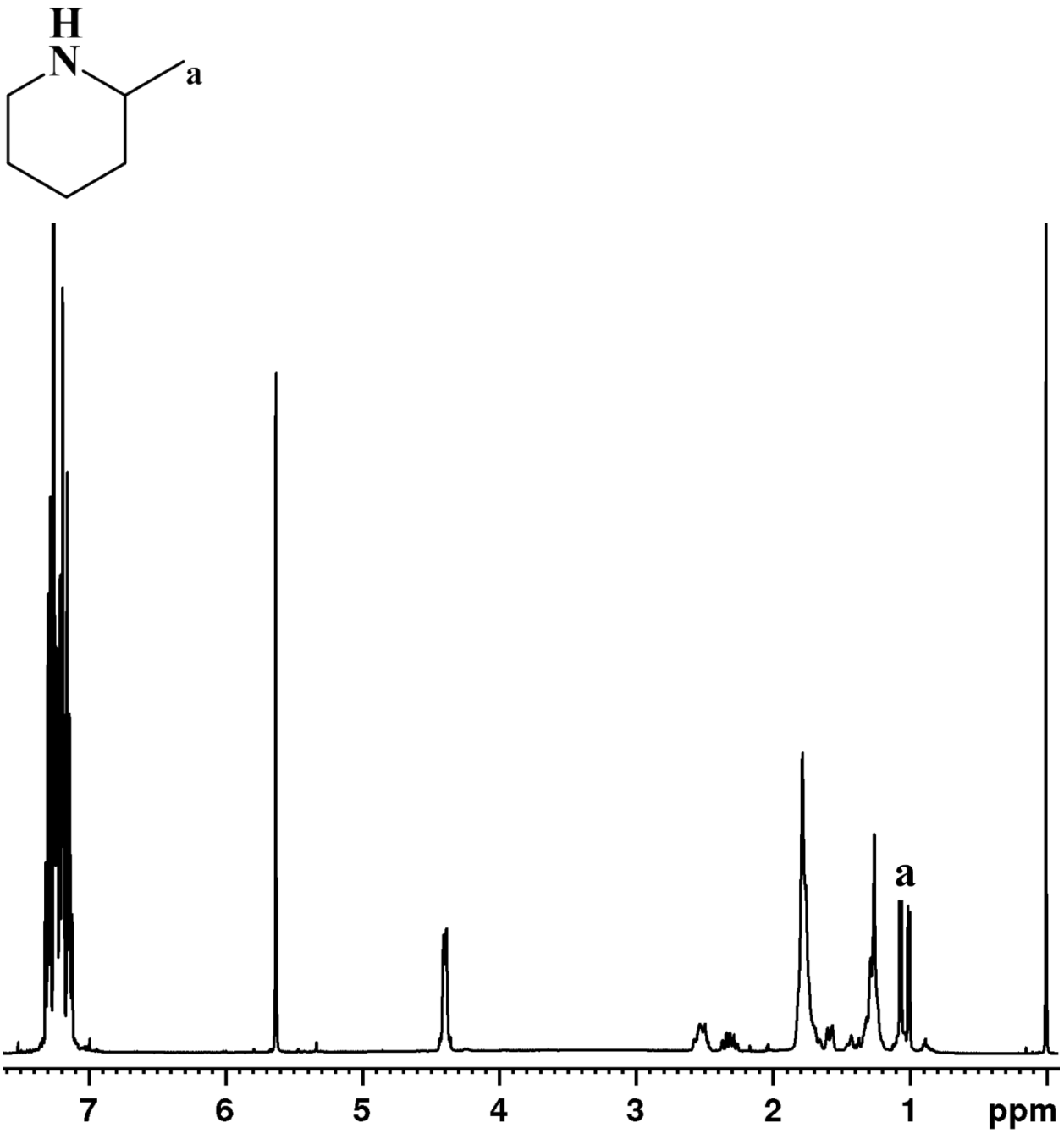


400 MHz ^{1}H-NMR spectrum of (*R/S*)-1-(p-tolyl)ethanamineand(*S*)-CBHA-DPA in $CDCl_3$

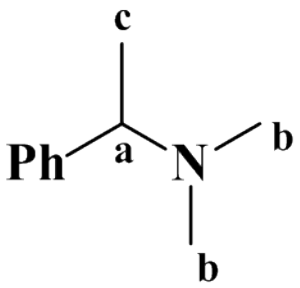


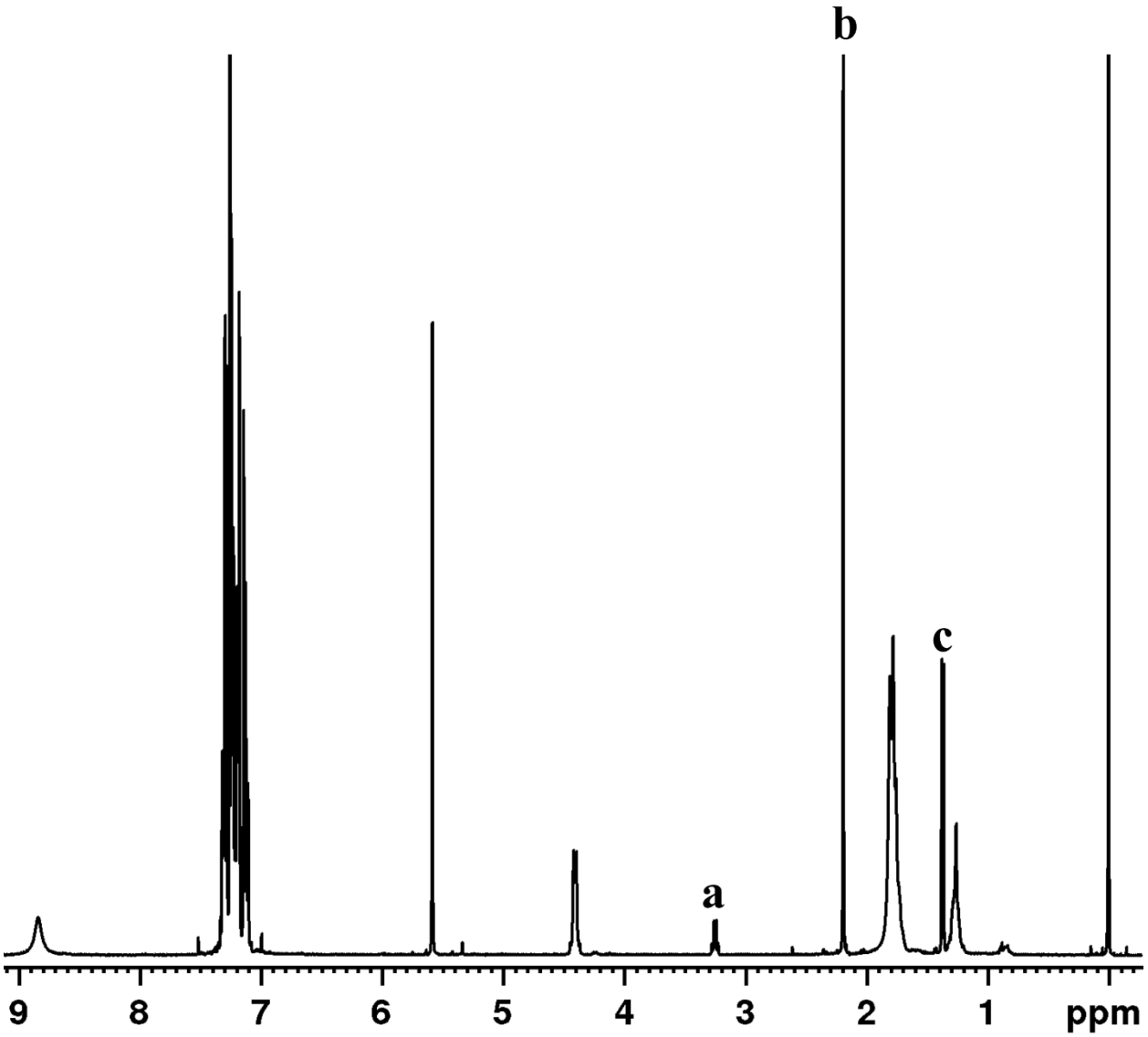


400 MHz ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine and (*S*)-CBHA-DPA in $CDCl_3$

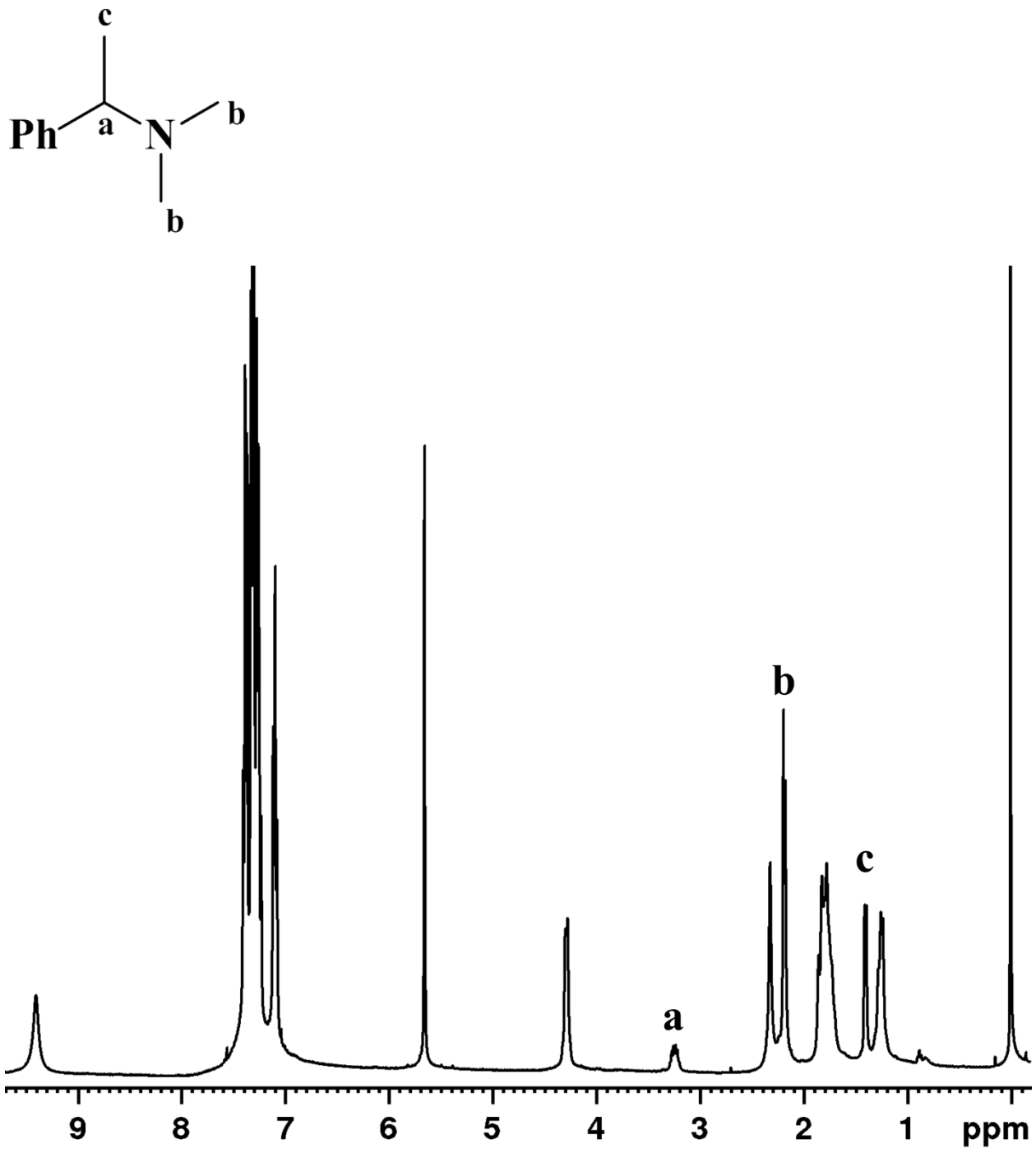


400 MHz ^{1}H -NMR spectrum of (*R/S*)–N,N dimethyl 1-phenyl ethylamine and (*S*)-CBHA-DPA in $CDCl_3$ at 298K

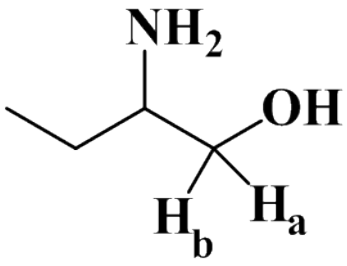


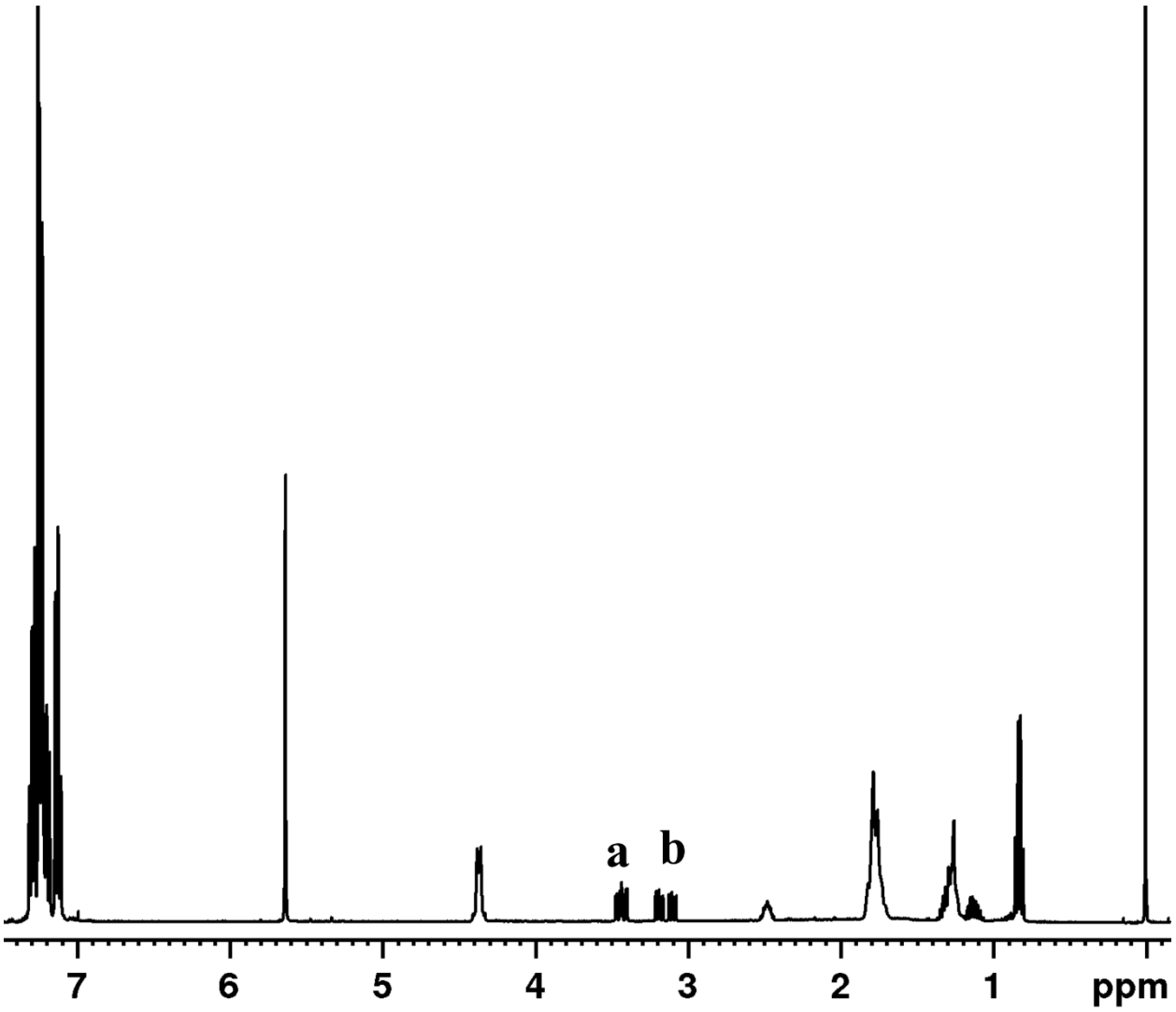


400 MHz ^{1}H -NMR spectrum of (*R/S*) – N,N dimethyl 1-phenyl ethylamine and (*S*)-CBHA-DPA in $CDCl_3$ at 233K

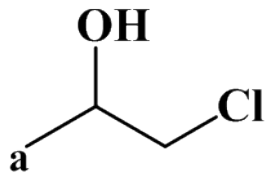


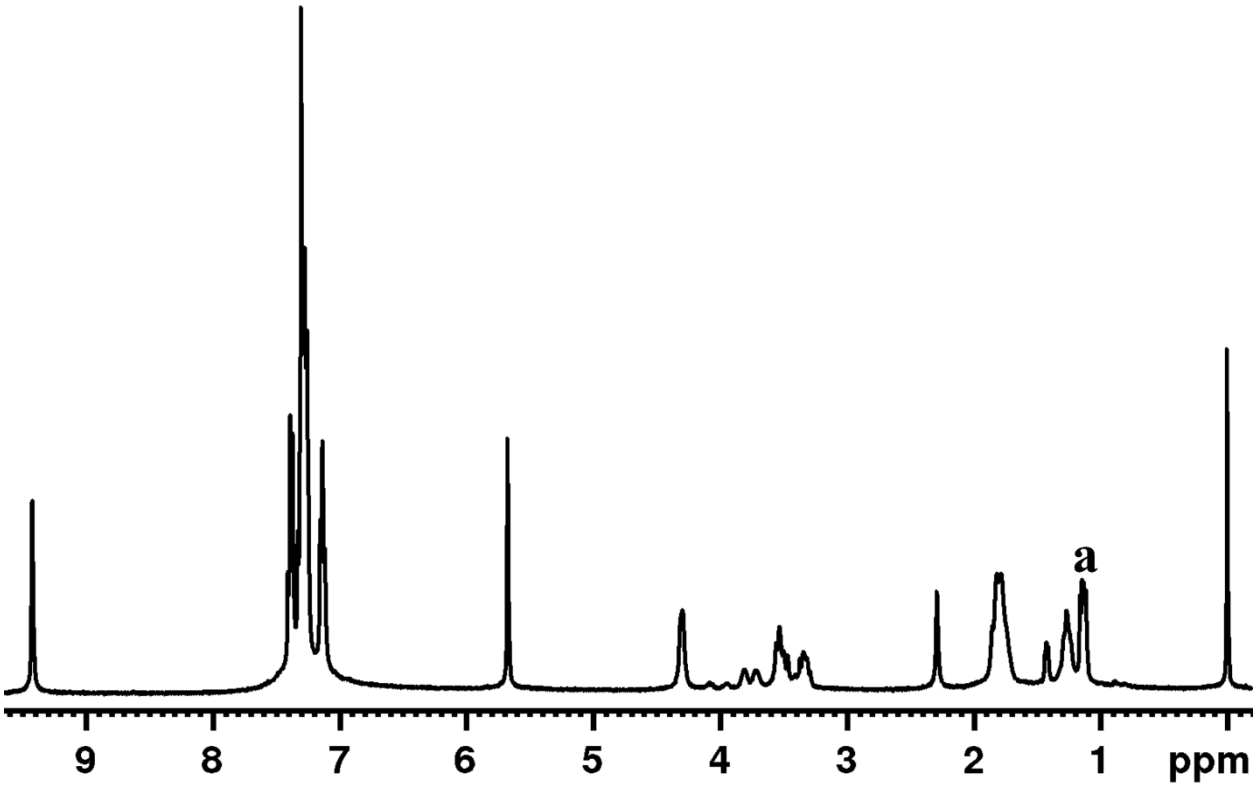
400 MHz ^{1}H -NMR spectrum of (*R/S*)– 2-Amino-1-butanol and (*S*)-CBHA-DPA in $CDCl_3$



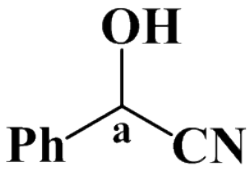


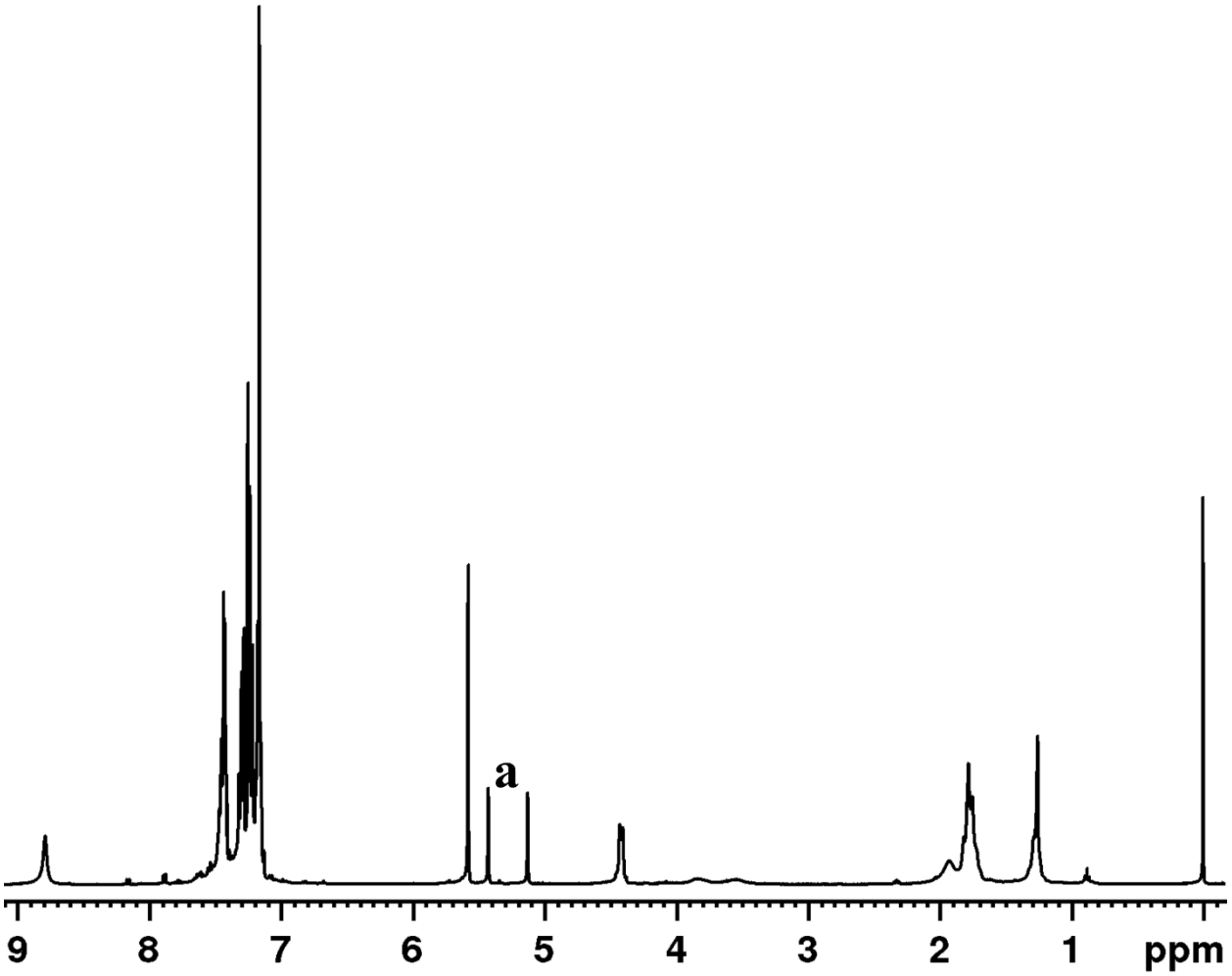
400 MHz ^{1}H -NMR spectrum of (*R/S*) –1-chloro 2-propanoland (*S*)-CBHA-DPA in $CDCl_3$ at 233K



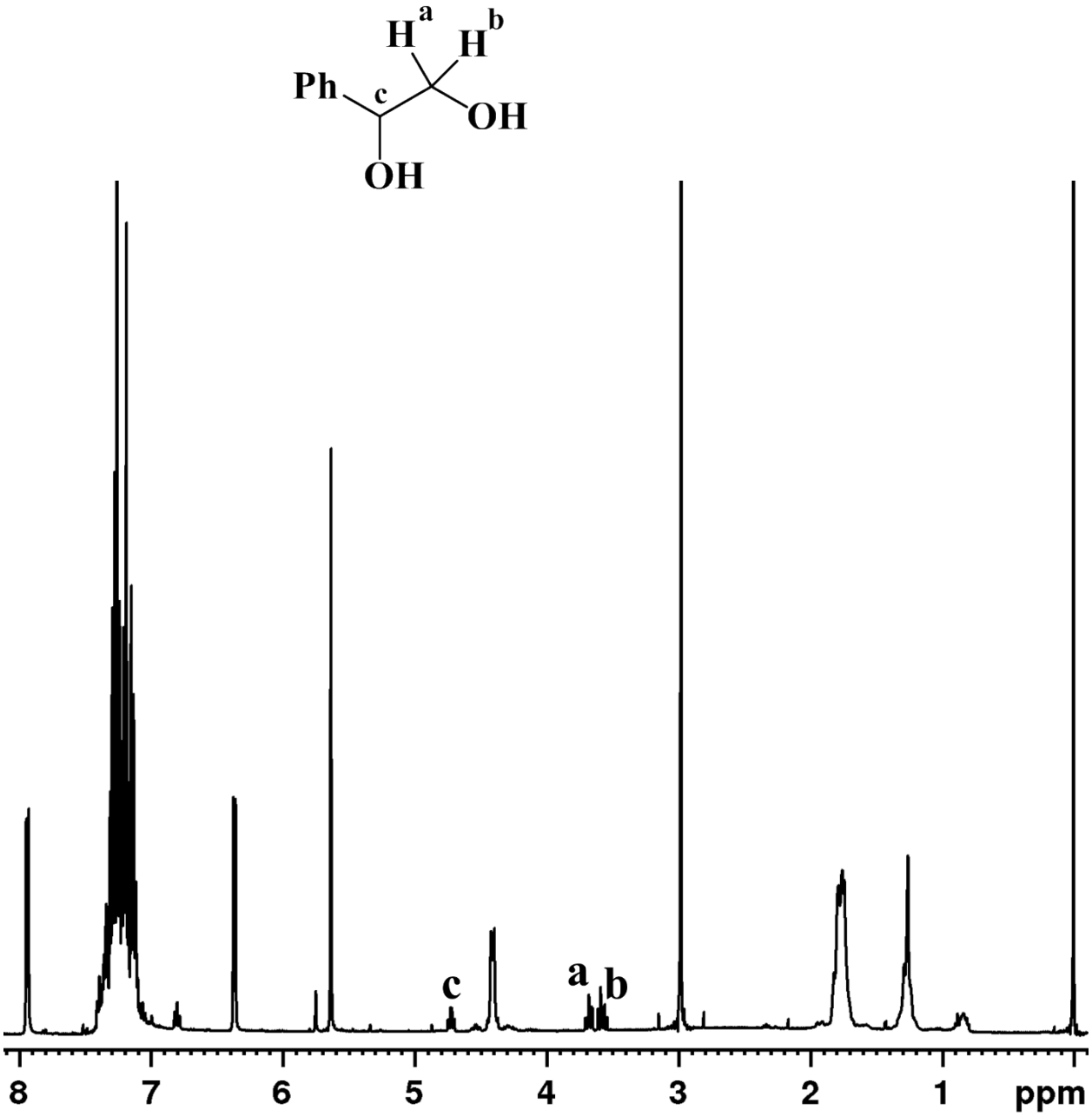


400 MHz ^{1}H -NMR spectrum of (*R/S*) –Mandelonitrile and (*S*)-CBHA-DPA in $CDCl_3$

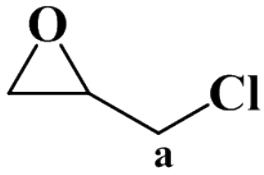


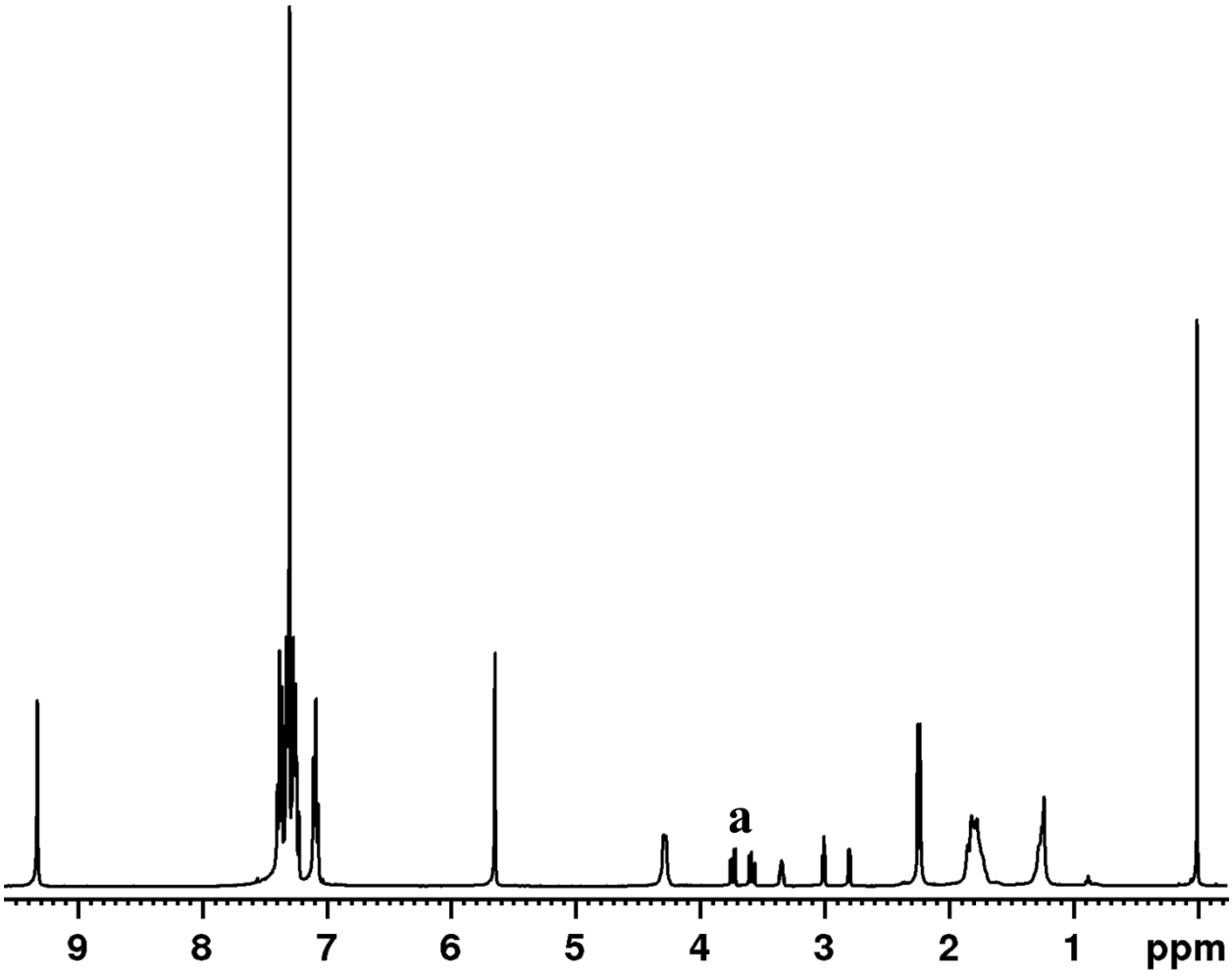


400 MHz ^{1}H -NMR spectra of (*R/S*)–1-Phenylethane-1, 2-diol , DMAP and (*S*)-CBHA-DPA in $CDCl_3$

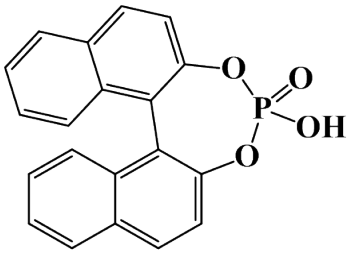


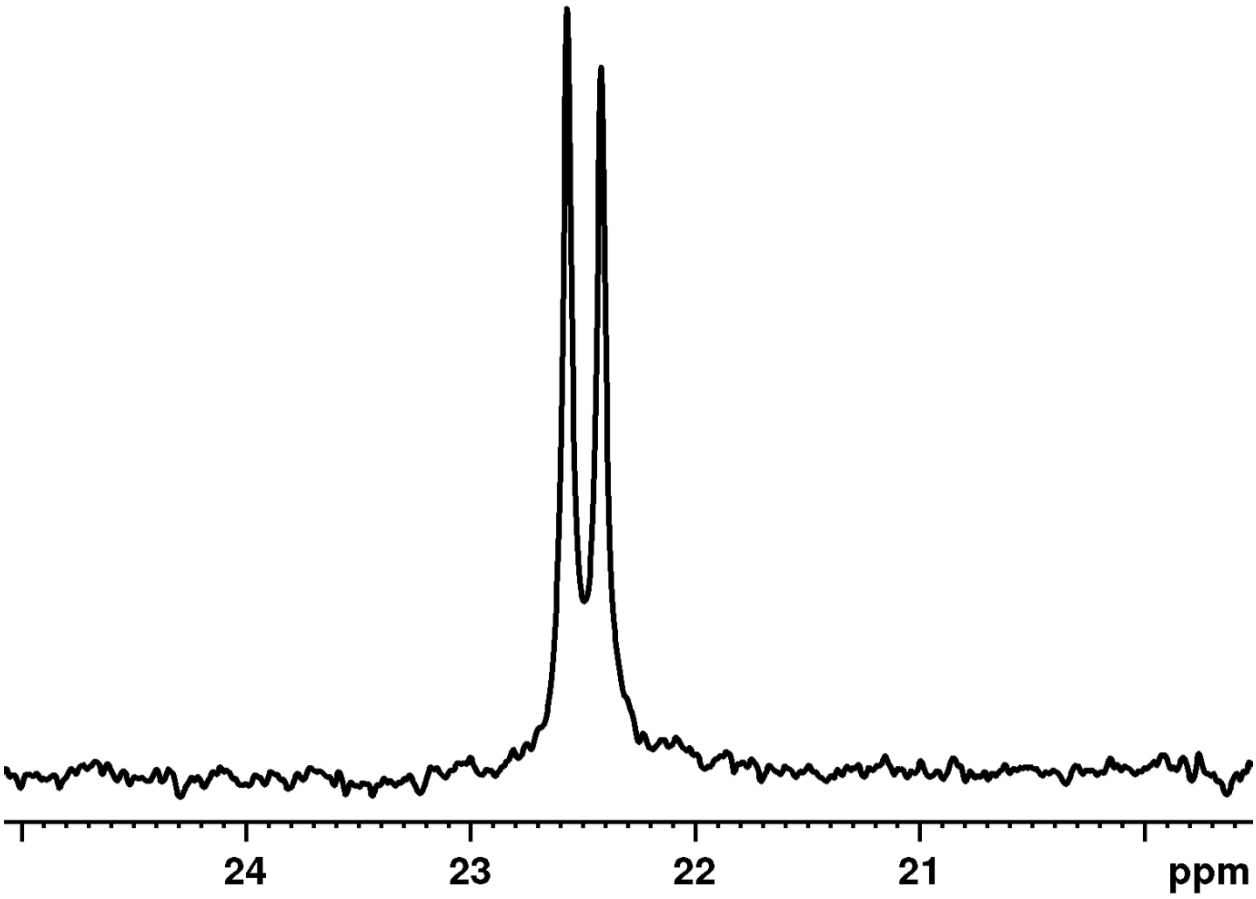
400 MHz ^{1}H -NMR spectrum of (*R/S*) –Epichlorohydrinand(*S*)-CBHA-DPA in $CDCl_3$ 233K



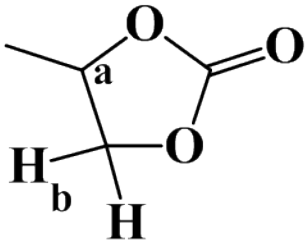


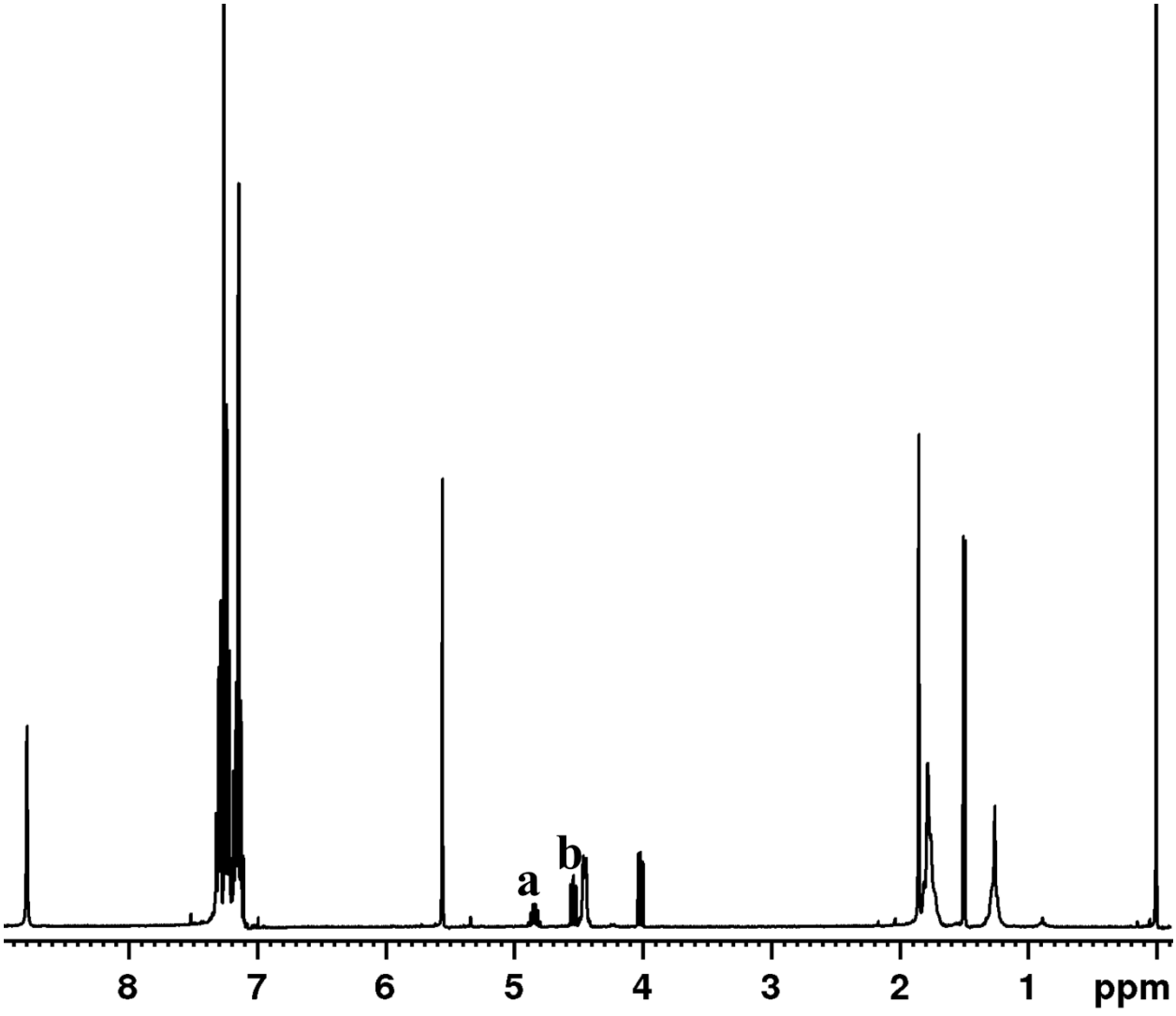
400 MHz ^{1}H -NMR spectra of (*R/S*) –1,1′-Binaphthyl-2,2′-diyl hydrogenphosphate , DMAP and (*S*)-CBHA-DPA in $CDCl_3$



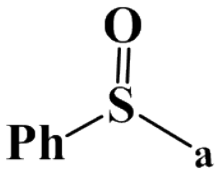


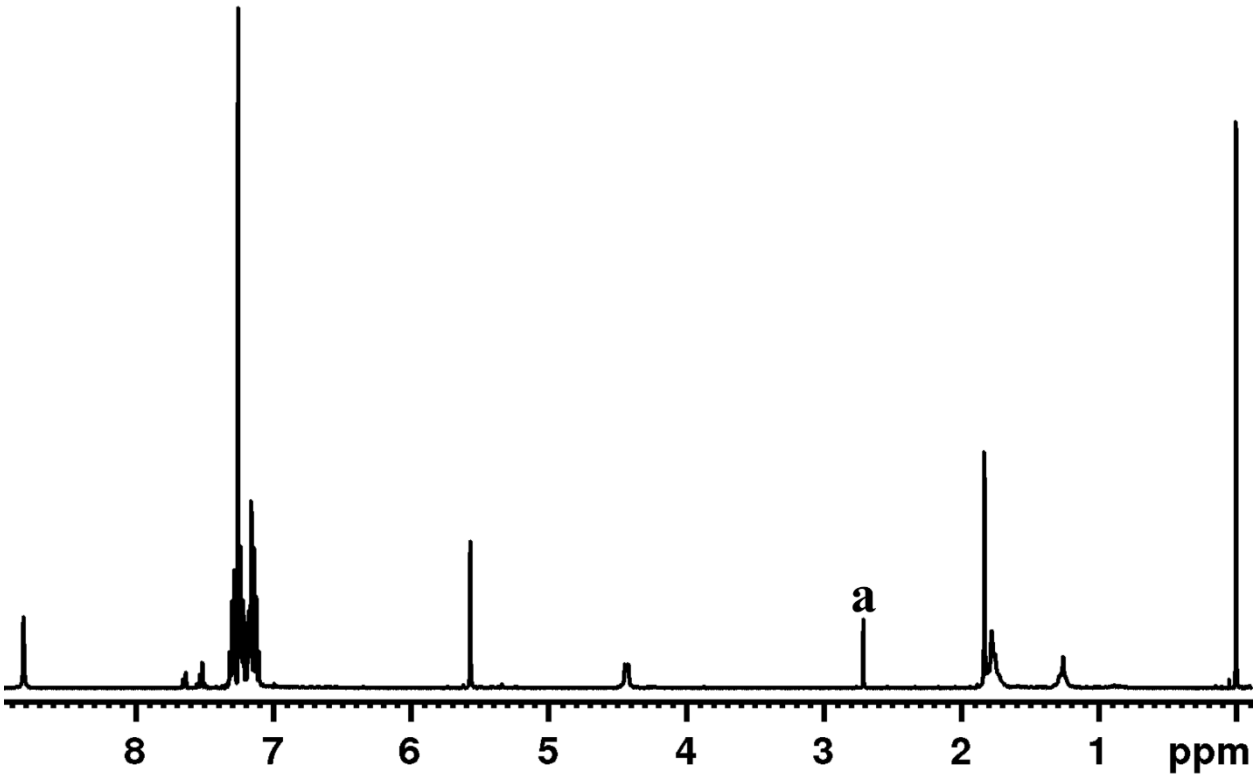
400 MHz ^{1}H -NMR spectrum of (*R/S*) – Propylene carbonate and (*S*)-CBHA-DPA in $CDCl_3$



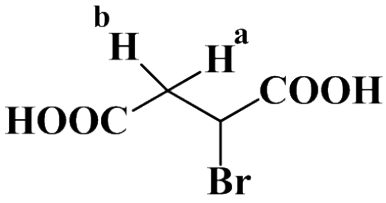


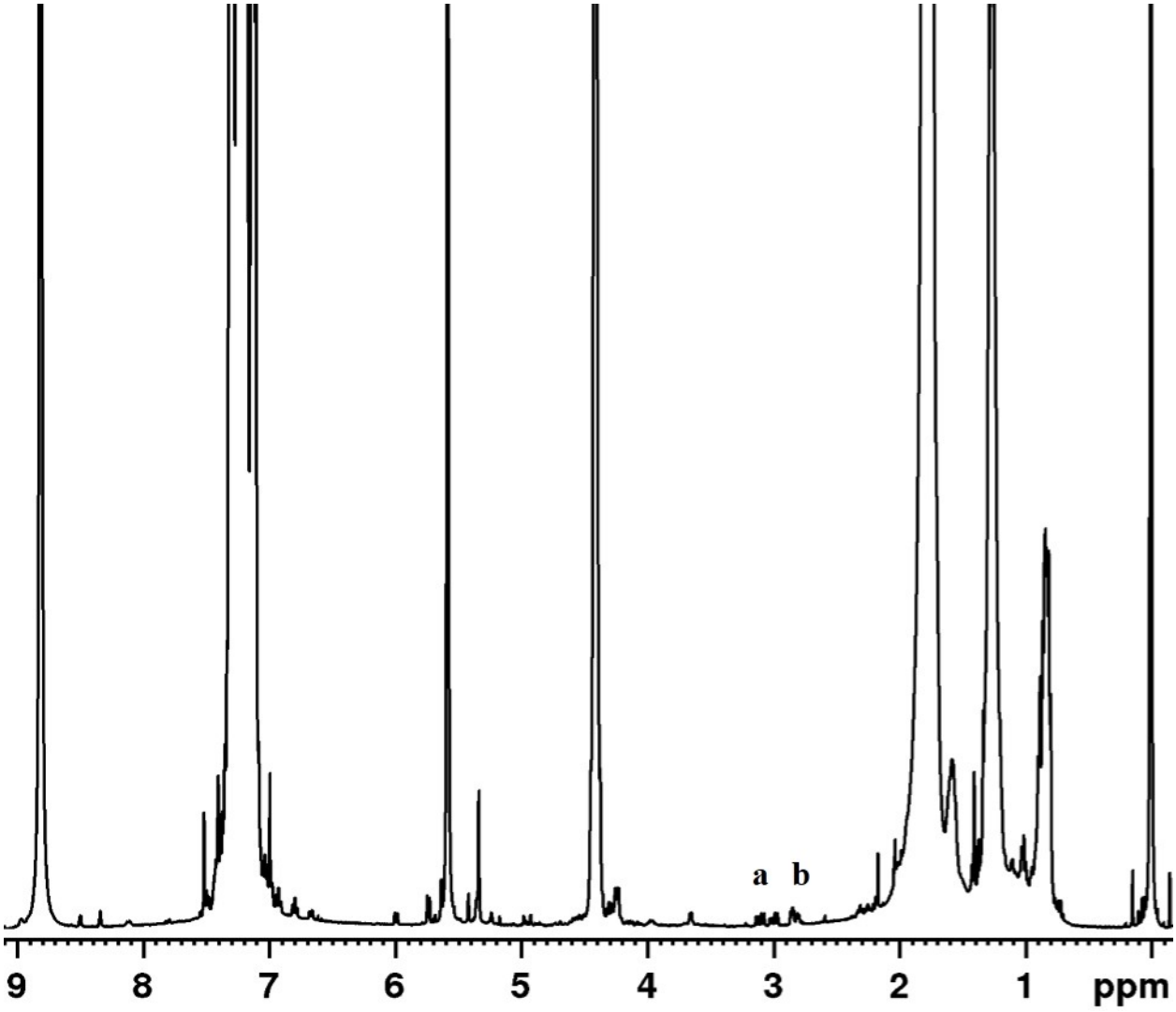
400MHz ^{1}H-NMR spectrum of (*R/S*) - Methyl phenyl sulfoxide and (*S*)-CBHA-DPA in $CDCl_3$





400 MHz ^{1}H-NMR spectrum of (*R/S*) - 2-bromosuccinic acid and (*S*)-CBHA-DPA in $CDCl_3$





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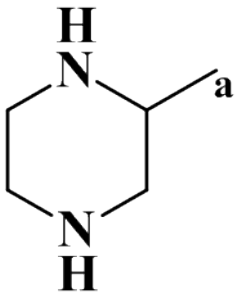

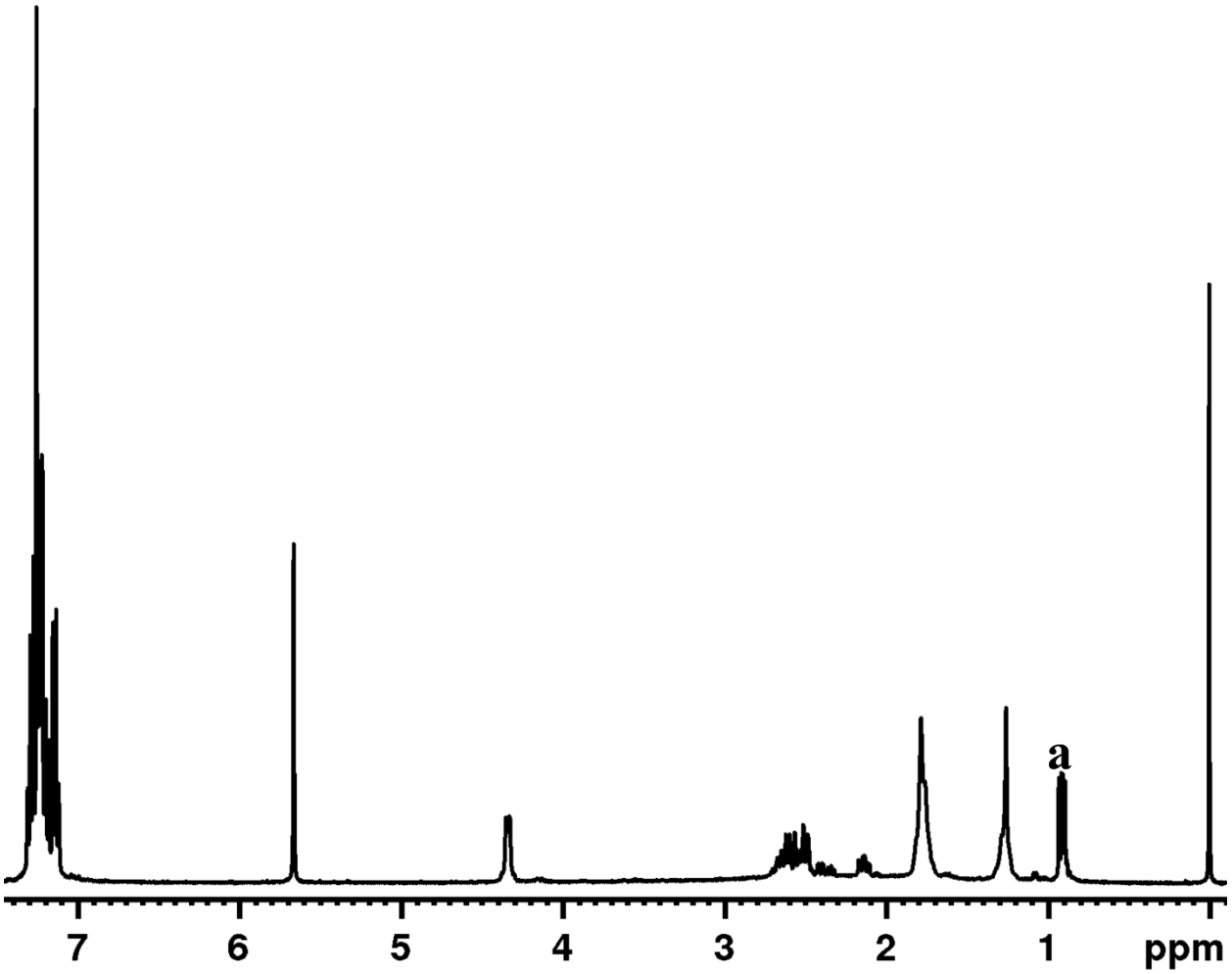

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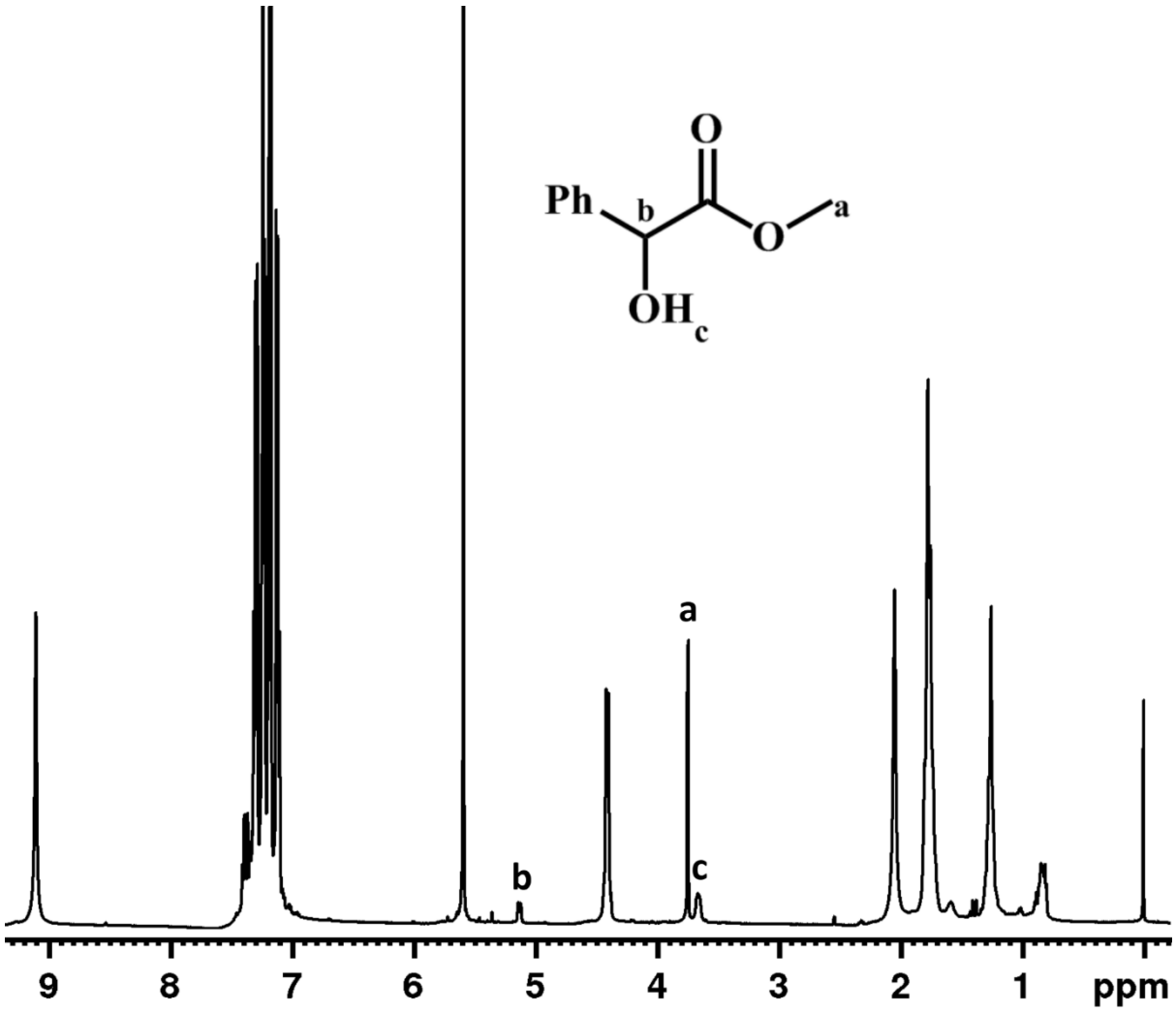
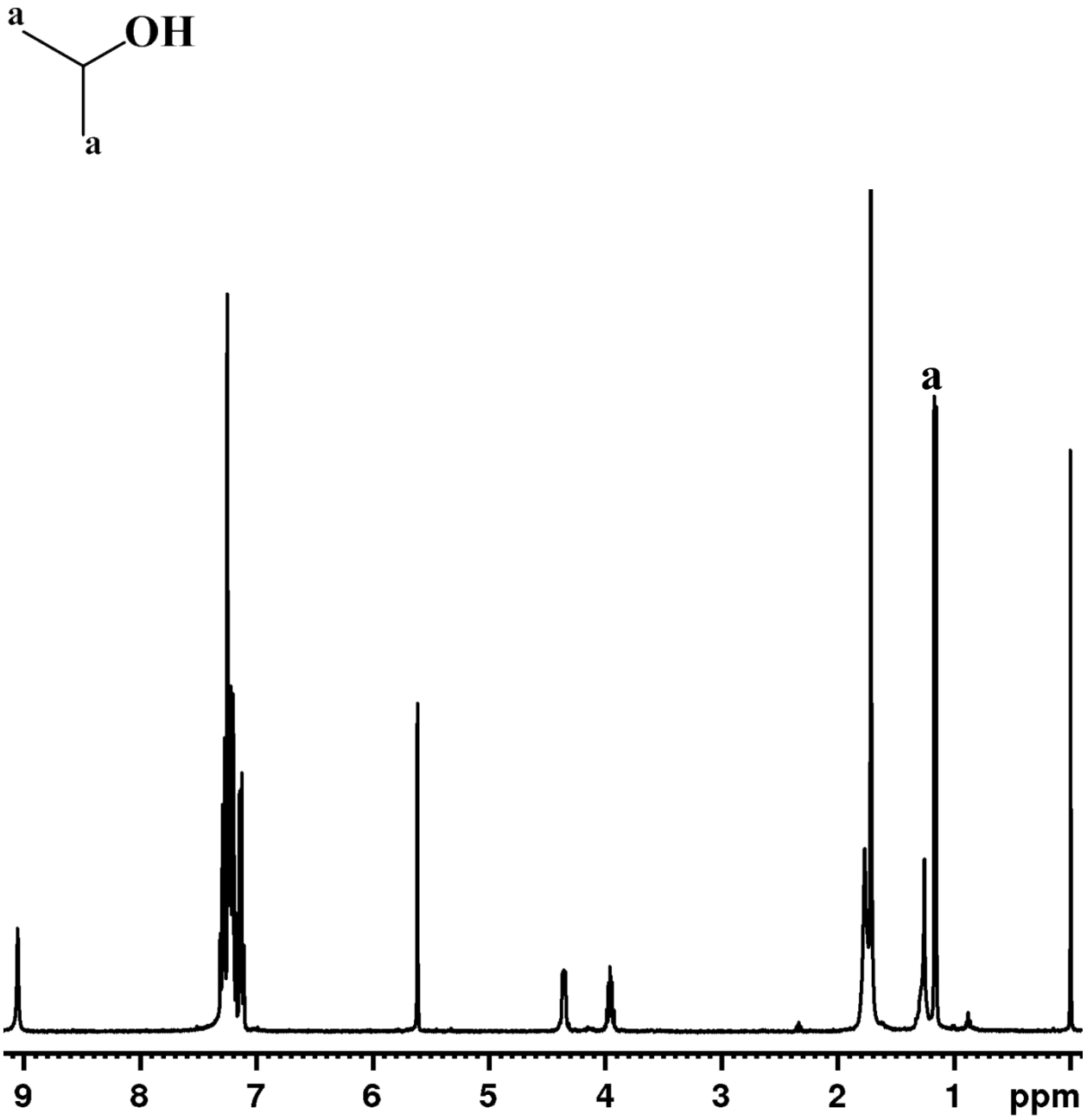
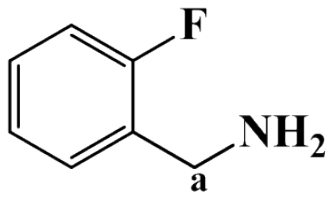
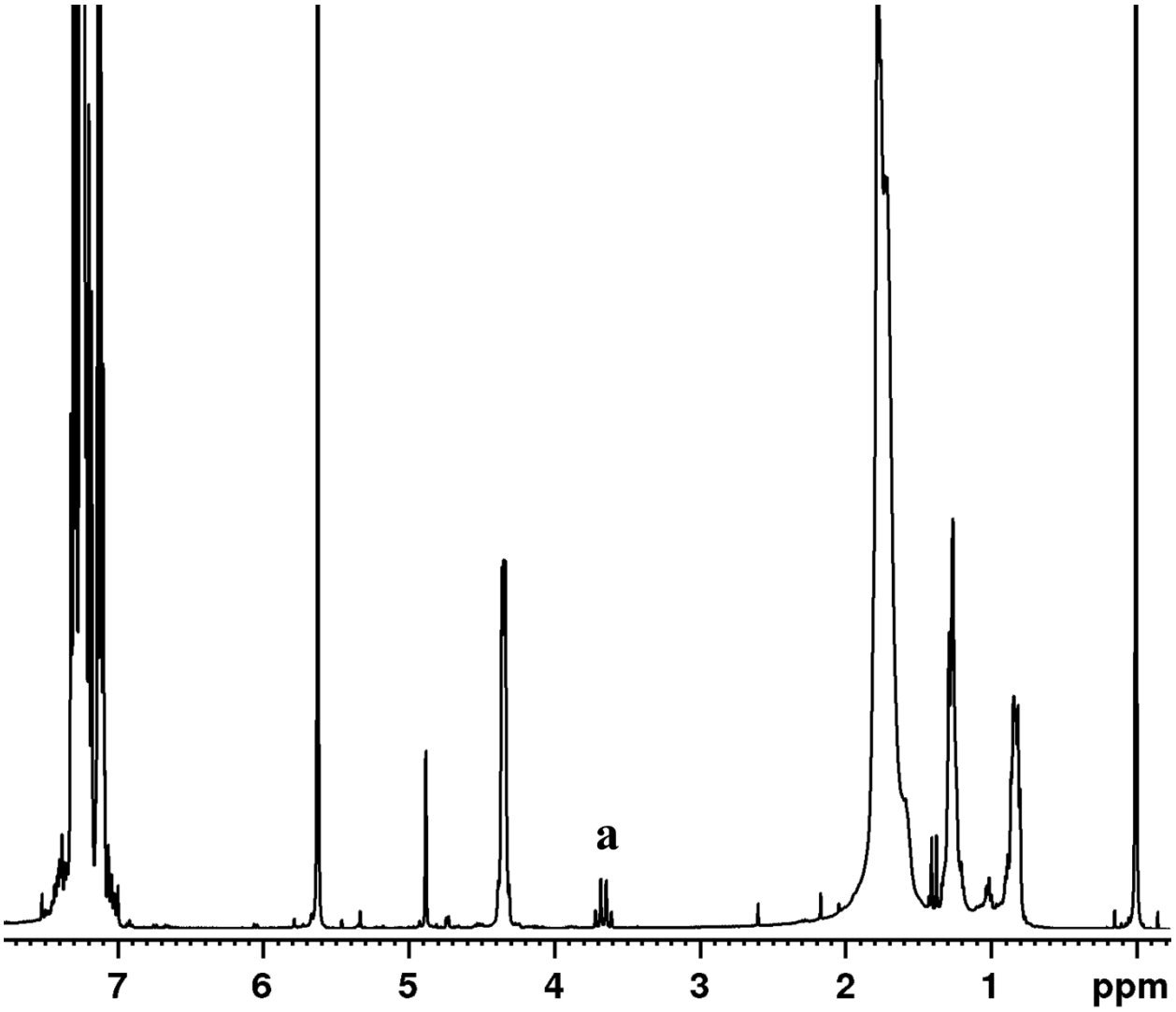


400 MHz ^{1}H -NMR spectrum of (*R/S*) – Isopropyl alcohol and (*S*)-CBHA-DPA in $CDCl_3$

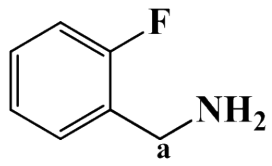


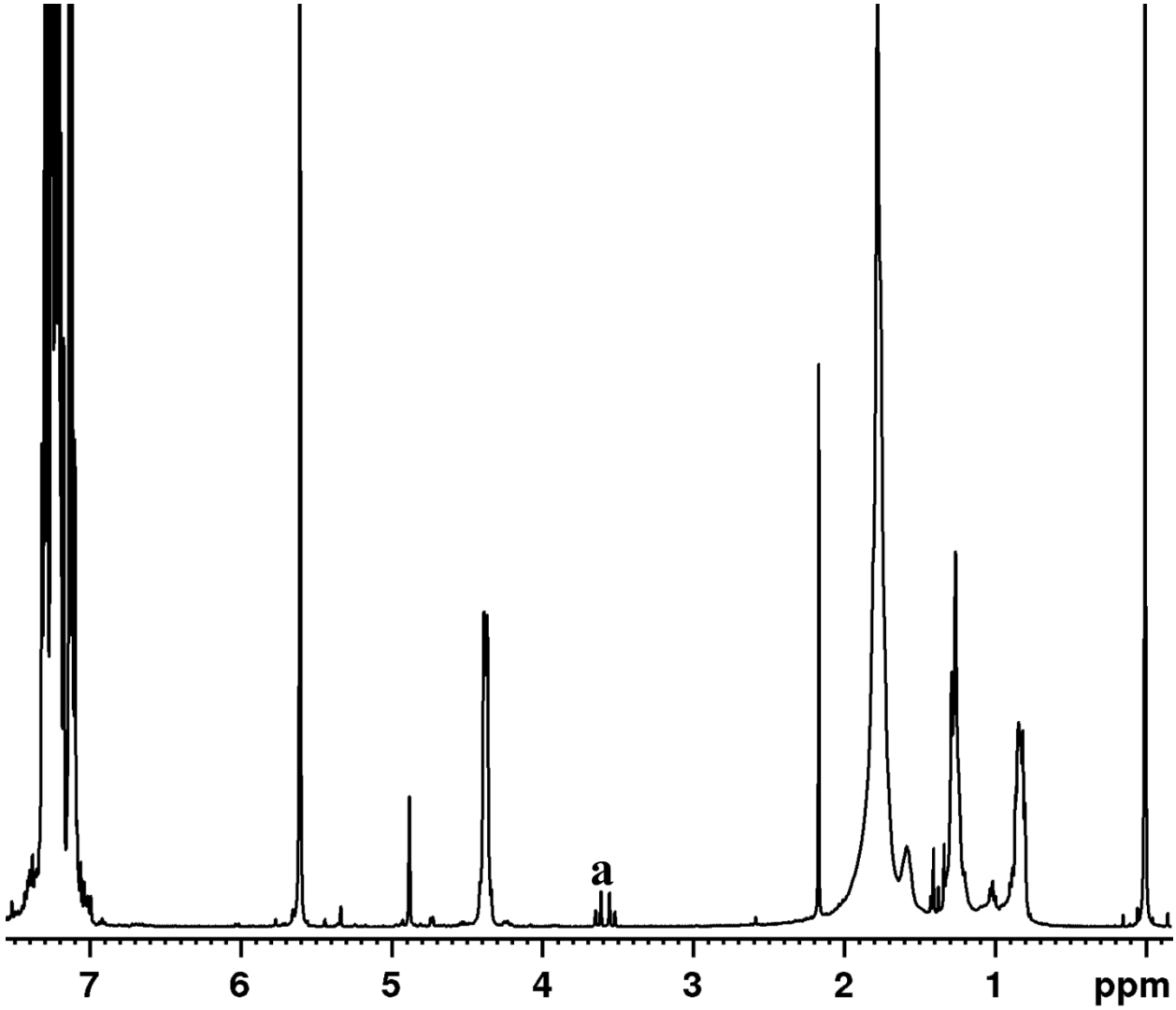
400 MHz ^{1}H -NMR spectrum of (*R/S*) – 2-fluoro benzyl amine and (*S*)-CBHA-DPA in $CDCl_3$



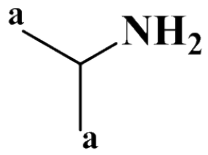


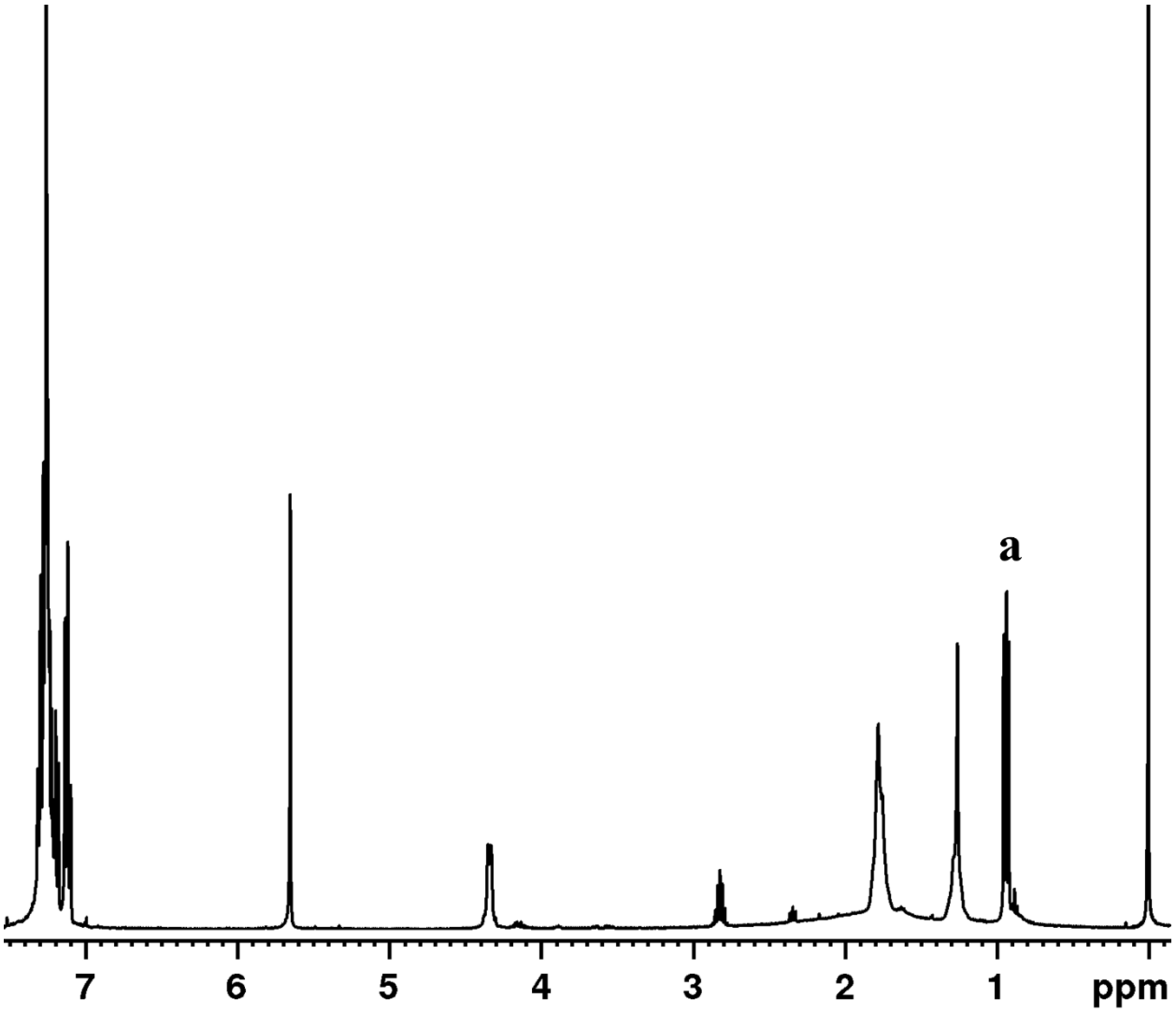
400 MHz ^{1}H -NMR spectrum of (*R/S*) – 2-fluoro benzyl amine and (*S*)-CBHA-DPA in $CDCl_3$ at 233K



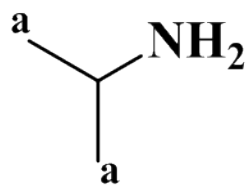


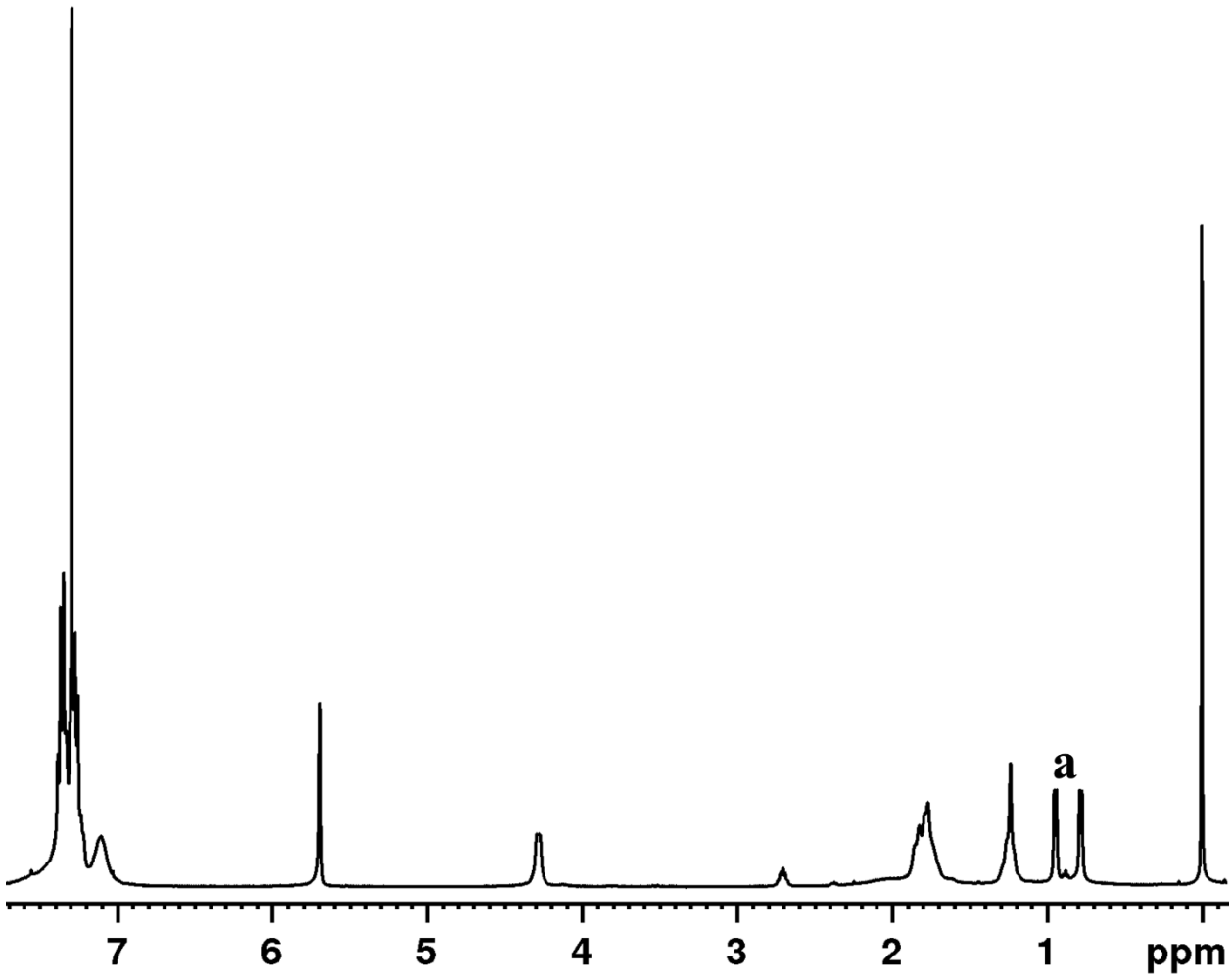
400 MHz ^{1}H -NMR spectrum of (*R/S*) – Isopropyl amineand(*S*)-CBHA-DPA in $CDCl_3$



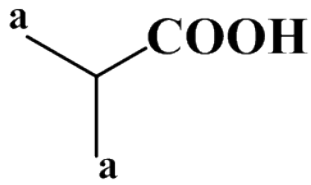


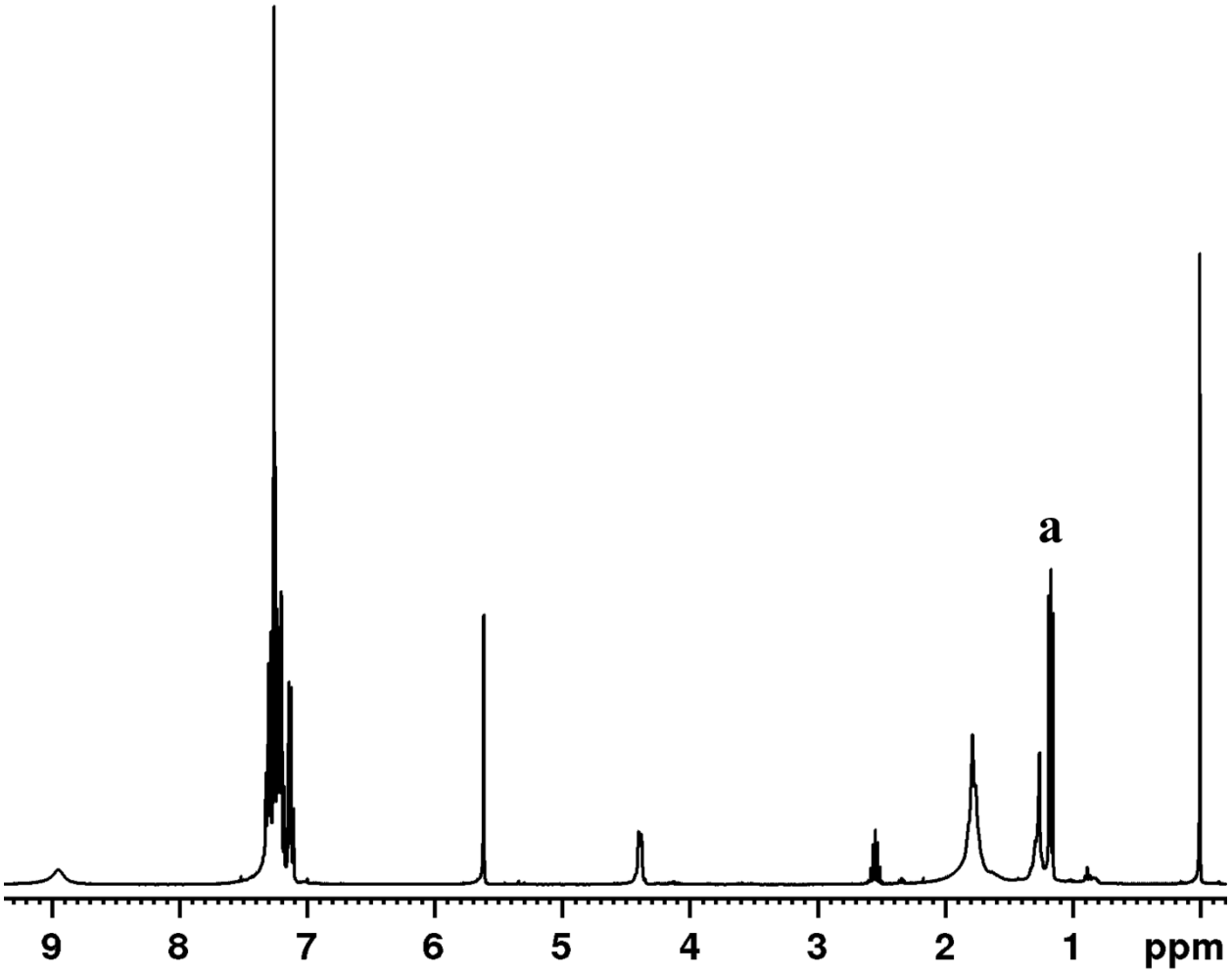
400 MHz ^{1}H -NMR spectrum of (*R/S*) – Isopropyl amine and (*S*)-CBHA-DPA in $CDCl_3$ at 233K



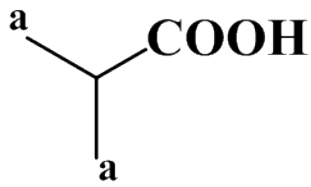


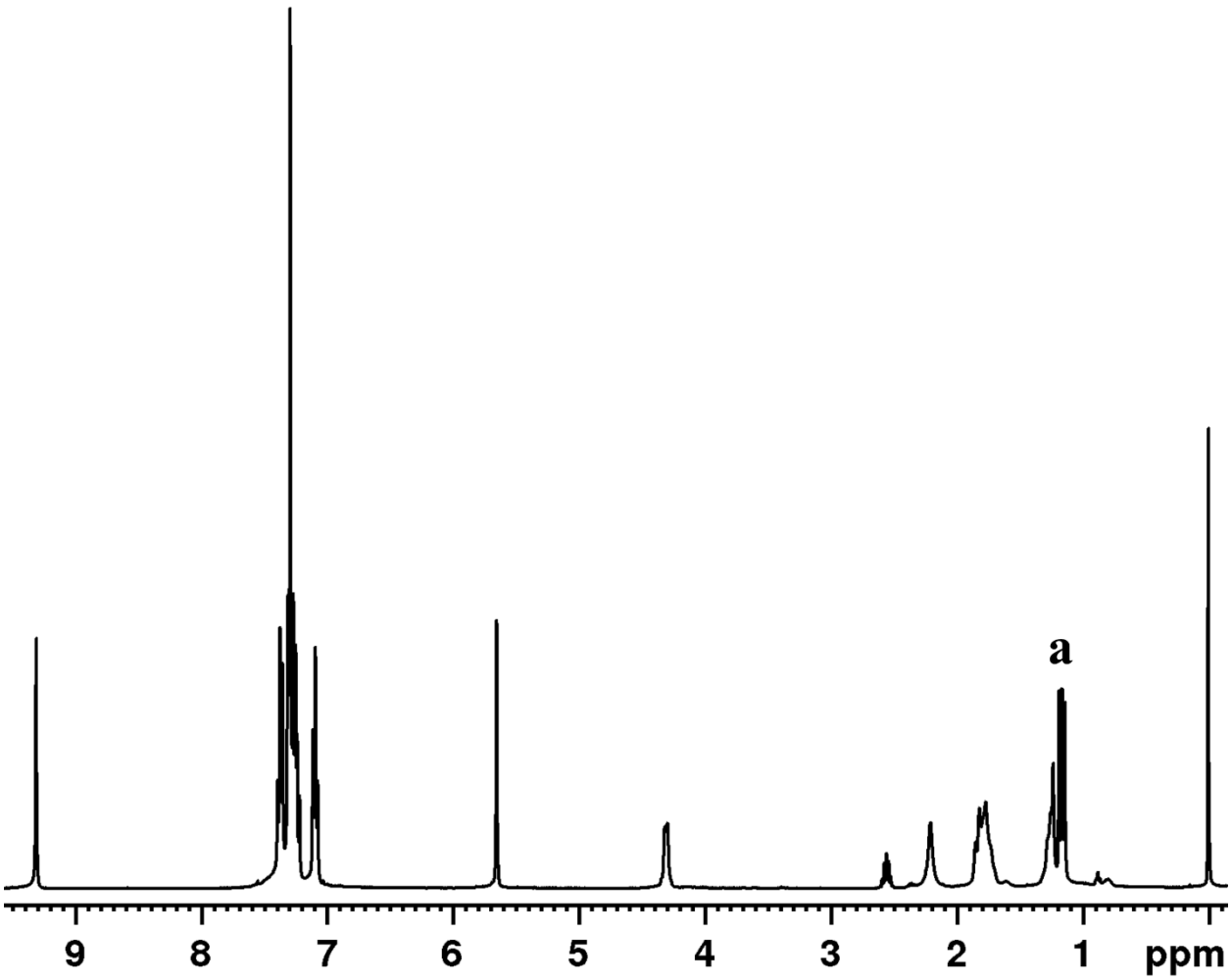
400 MHz ^{1}H -NMR spectrum of (*R/S*) – Isobutyric acid and (*S*)-CBHA-DPA in $CDCl_3$



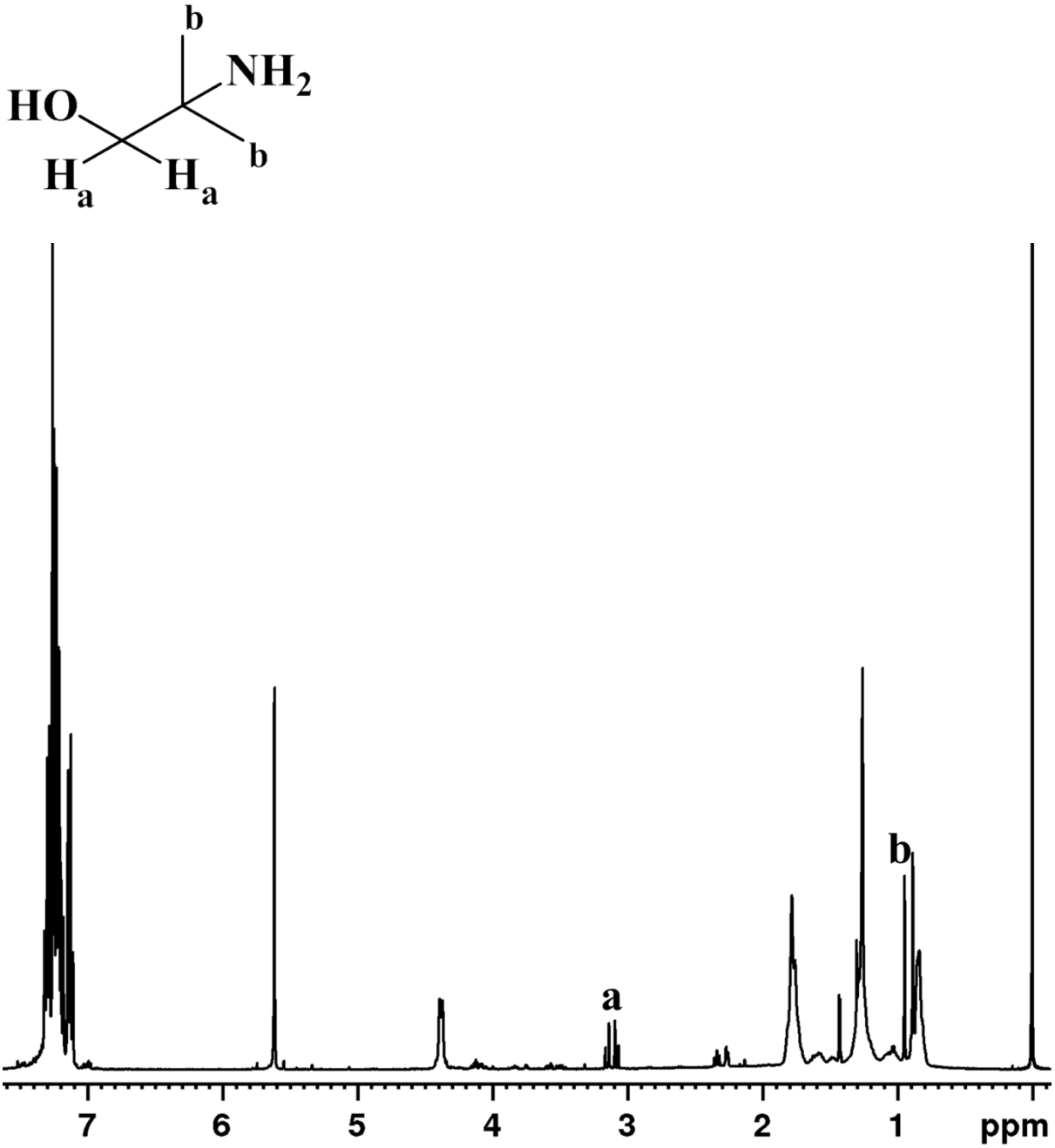


400 MHz ^{1}H -NMR spectrum of (*R/S*) – Isobutyric acid and (*S*)-CBHA-DPA in $CDCl_3$ at 233K

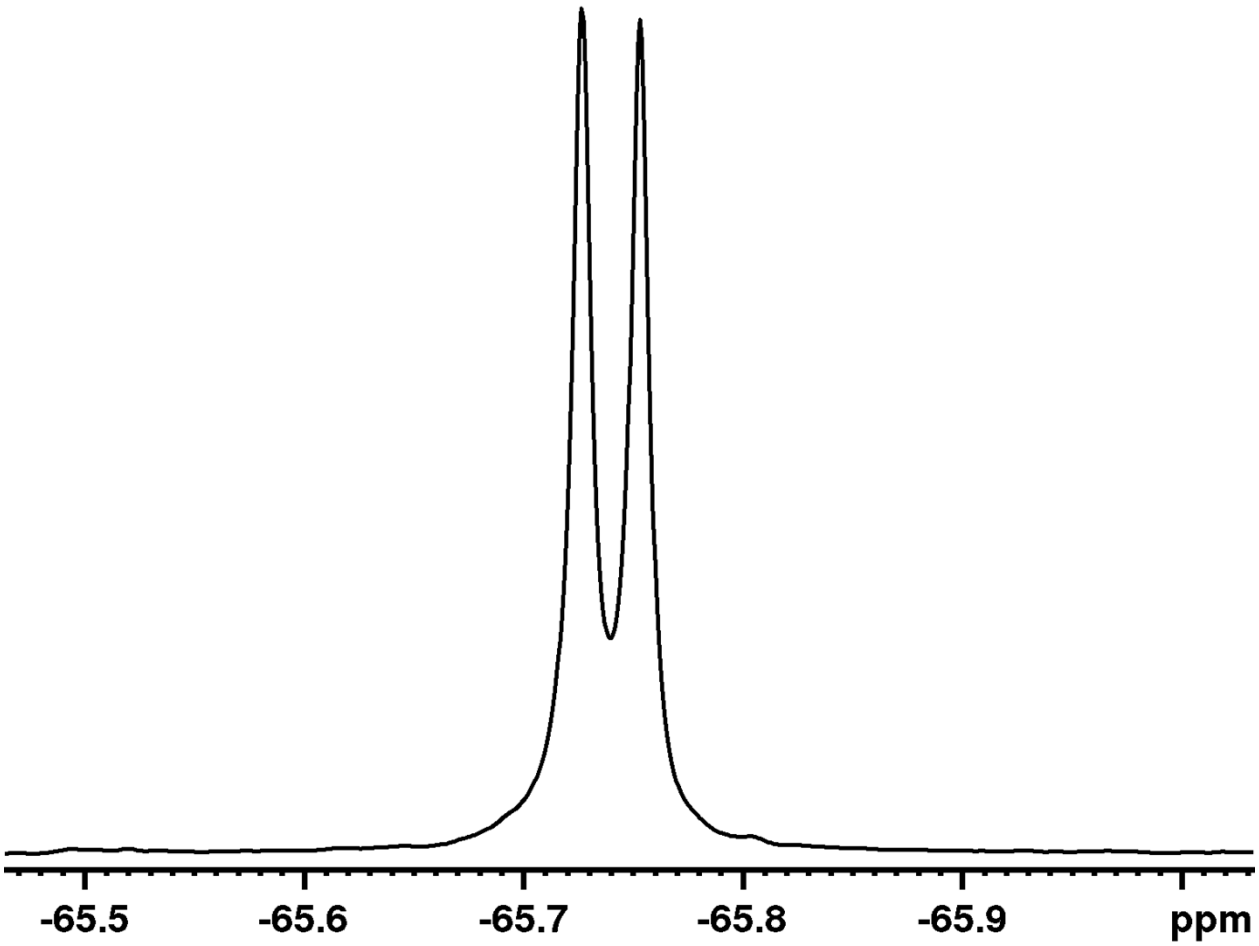




400 MHz ^{1}H -NMR spectrum of (*R/S*) – 2-Amino-2-methyl-1-propanol and (*S*)-CBHA-DPA in $CDCl_3$



^{19}F -NMR spectrum of (*R/S*) – 4-(Trifluoromethyl)mandelic acid and (*S*)-CBHA-DPA in $CDCl_3$



^{13}C –NMR spectrum of (*R/S*) – Mandelonitrile and(*S*)-CBHA-DPA in $CDCl_3$

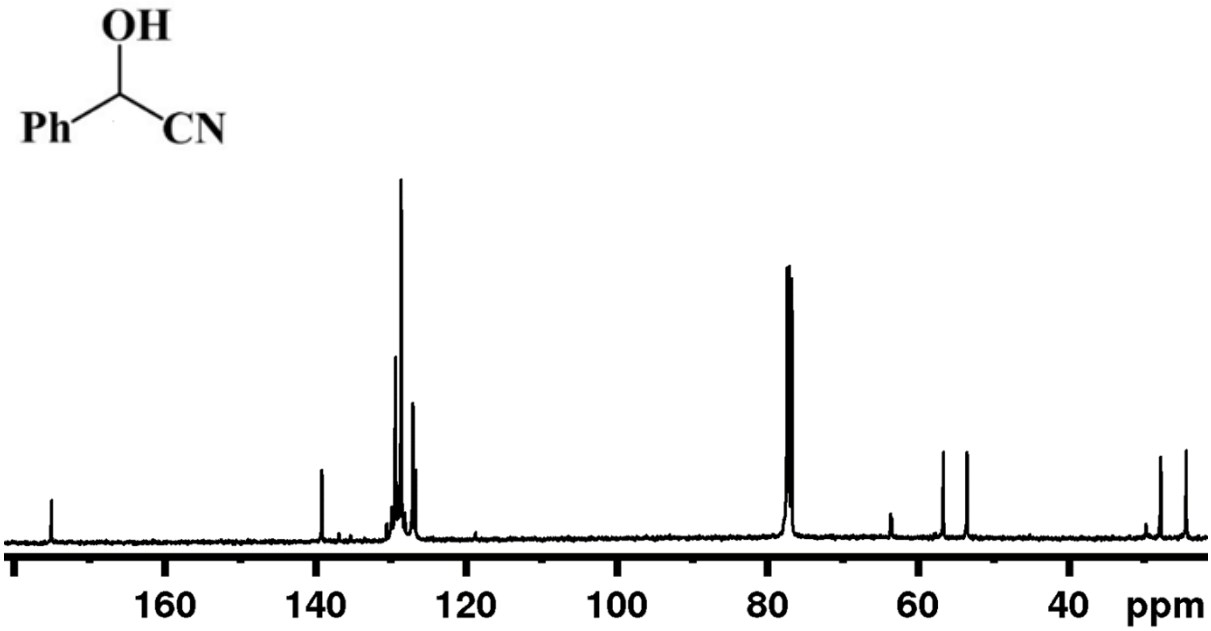
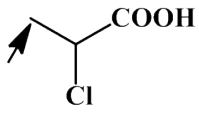
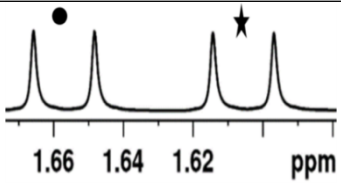
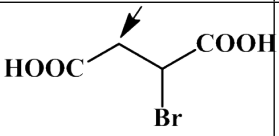
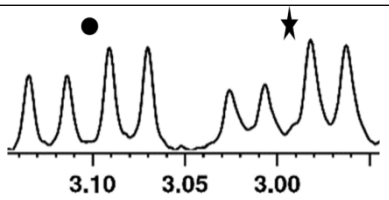
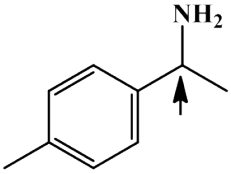
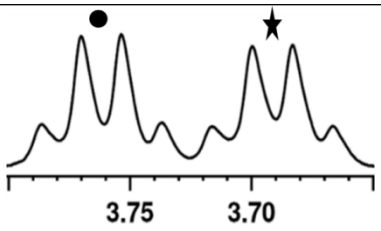
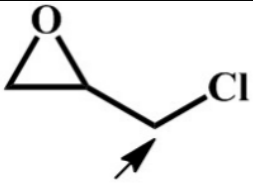
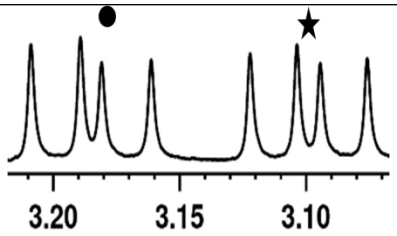
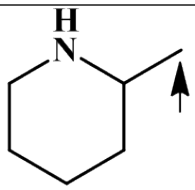
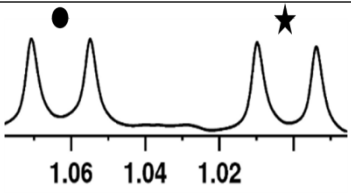
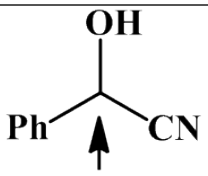
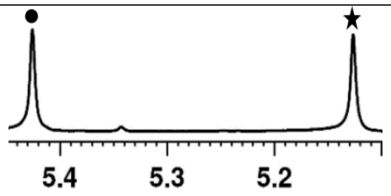
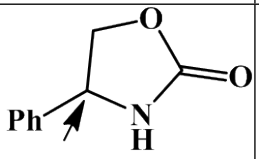
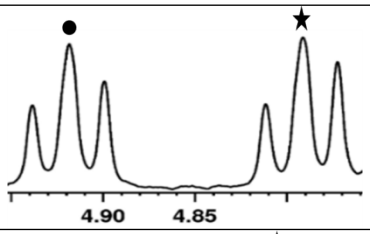
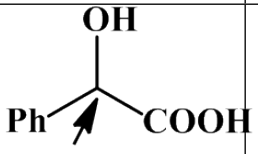
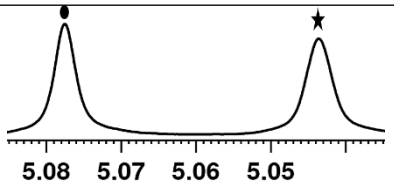
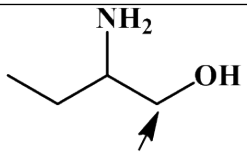
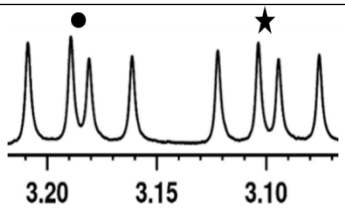
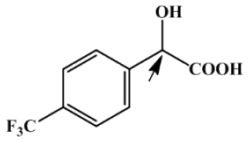
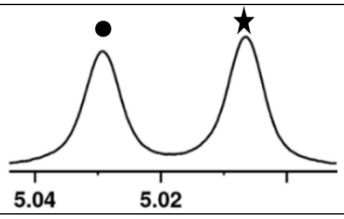
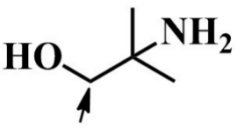
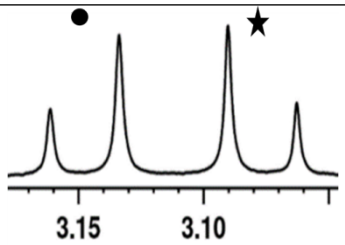
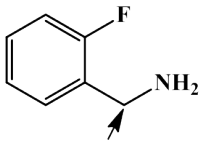
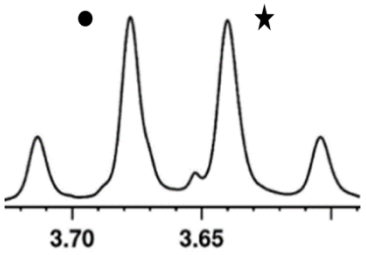
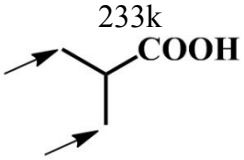
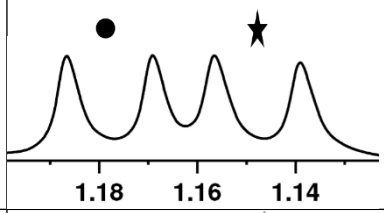
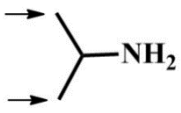
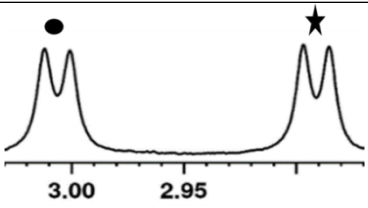
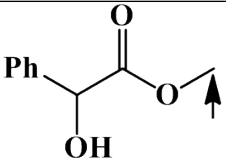
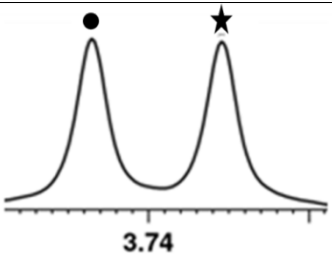
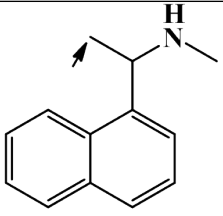
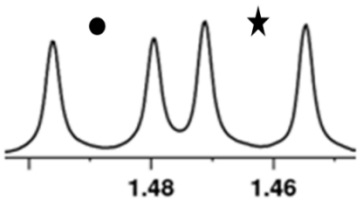
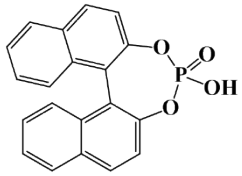
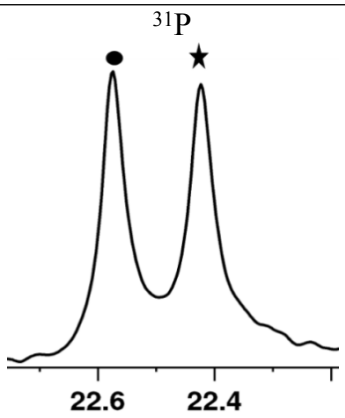
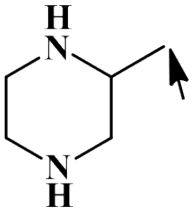
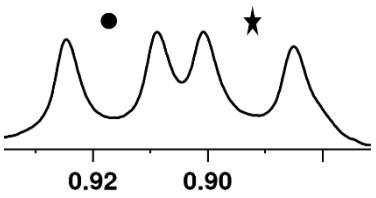
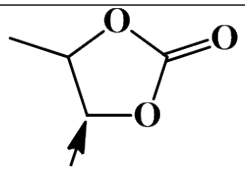
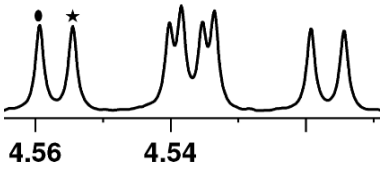
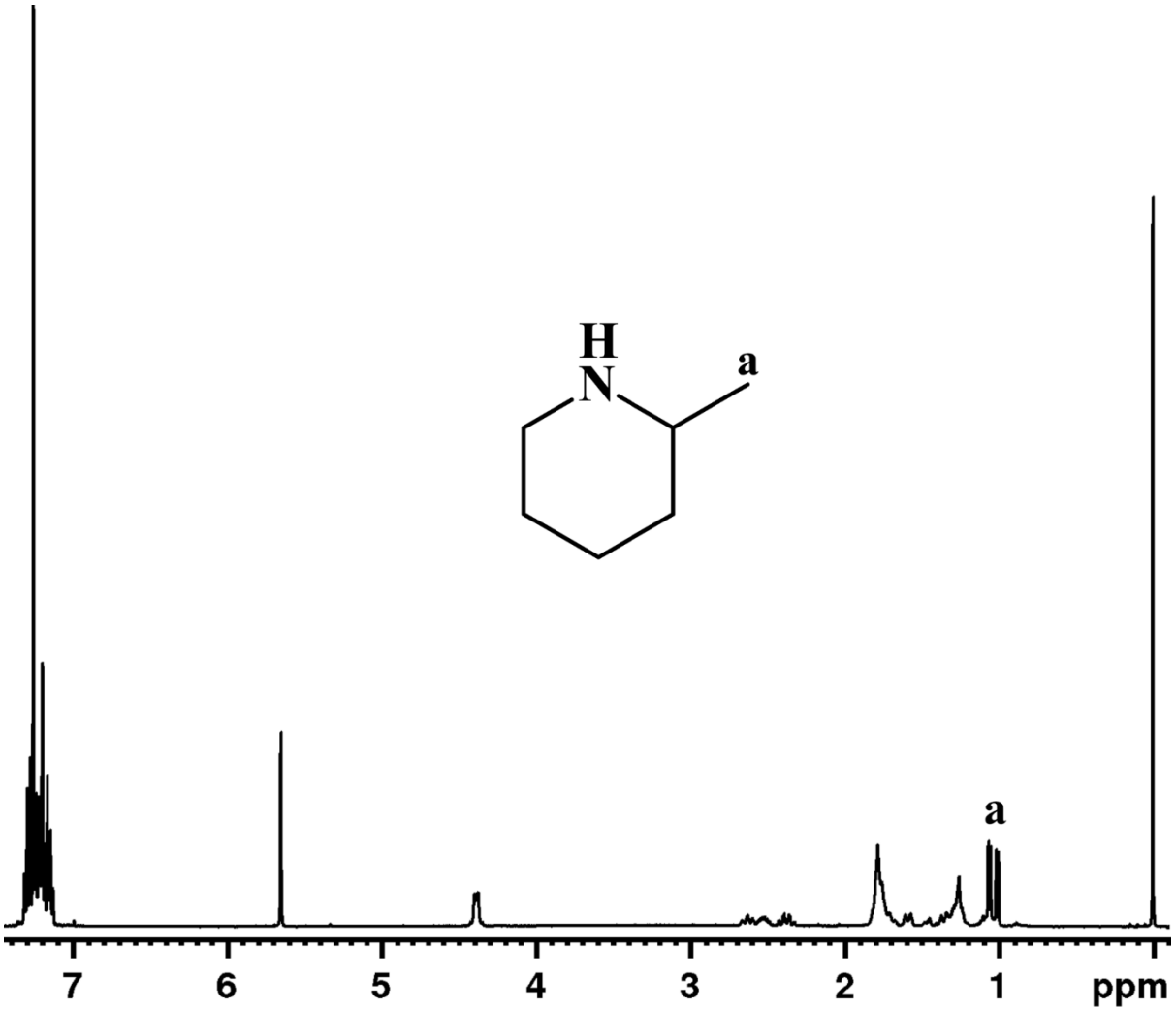


Table:^{1}H-NMR spectrum pertaining to a specific proton of different chiral analytes showing discrimination and their chemical structure

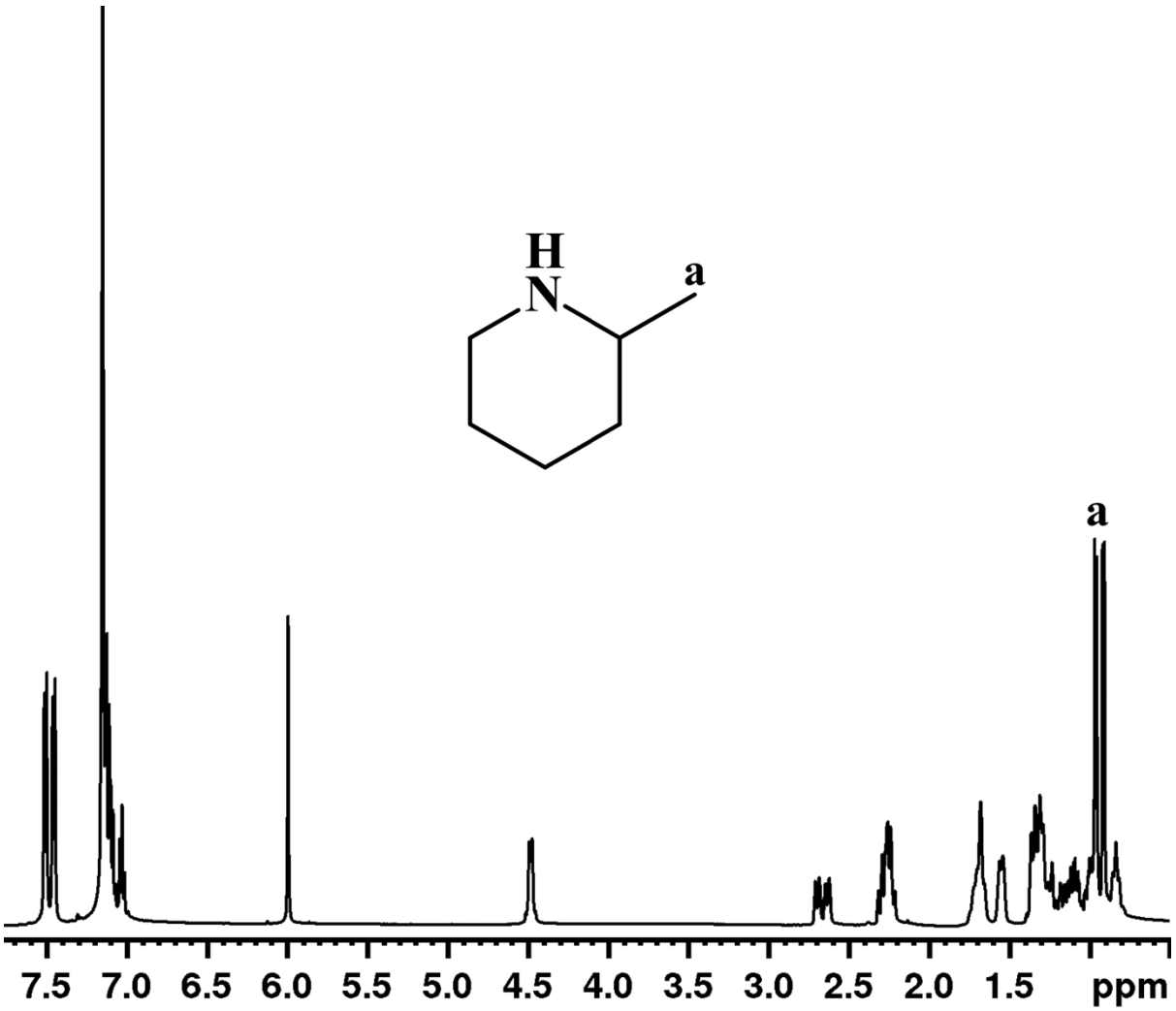
Entry	Guest	Spectrum	Entry	Guest	Spectrum
1			2		
3			4	 233K	
5			6		
7			8		
9			10		
11			12		
13	233k 		14	 233k	
15			16		

17			18		
19					

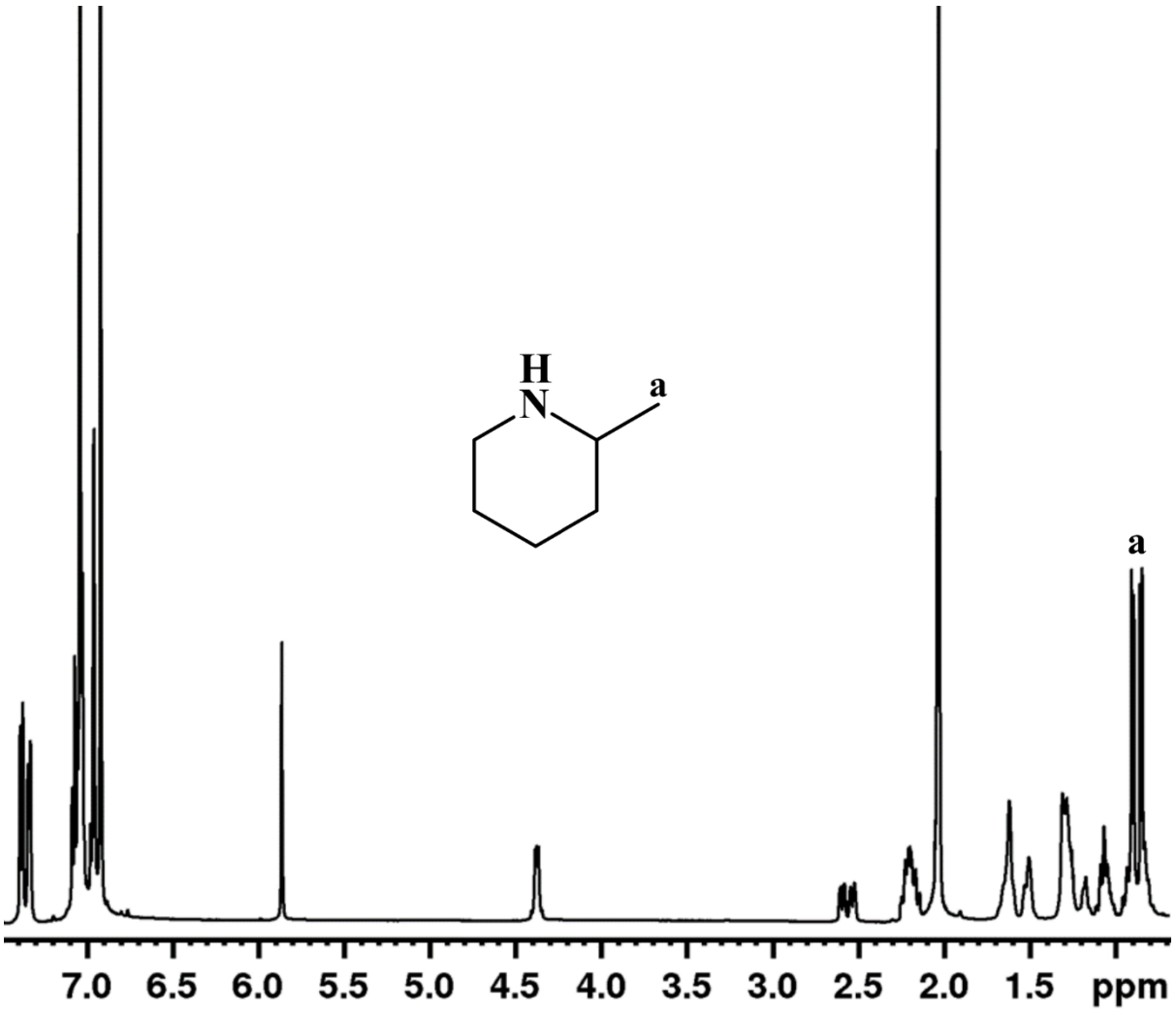
400MHz ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine and (*S*)-CBHA-DPA (1:2) in $CDCl_3$



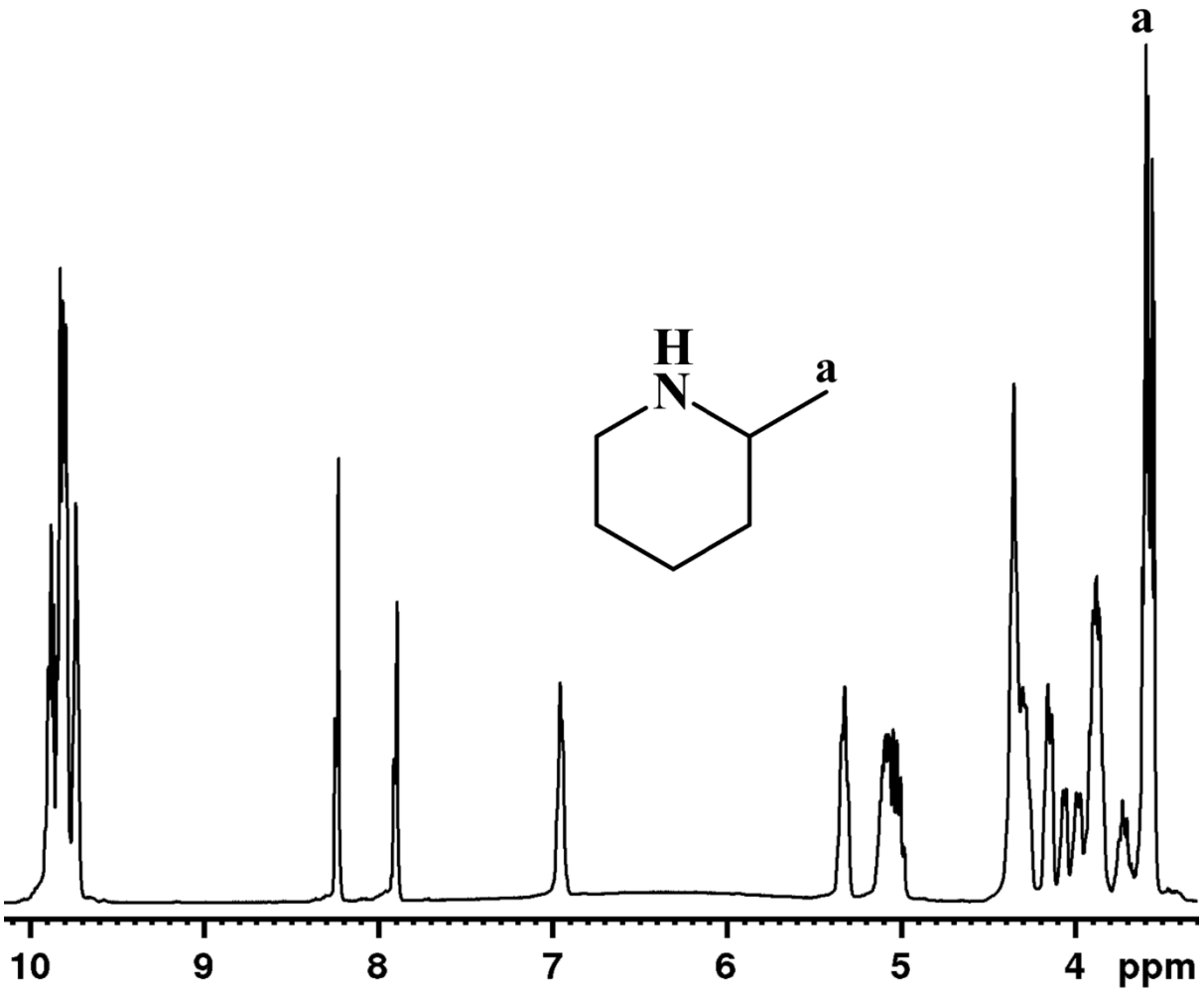
500MHz ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine and (*S*)-CBHA-DPA (1:2) in C_6D_6



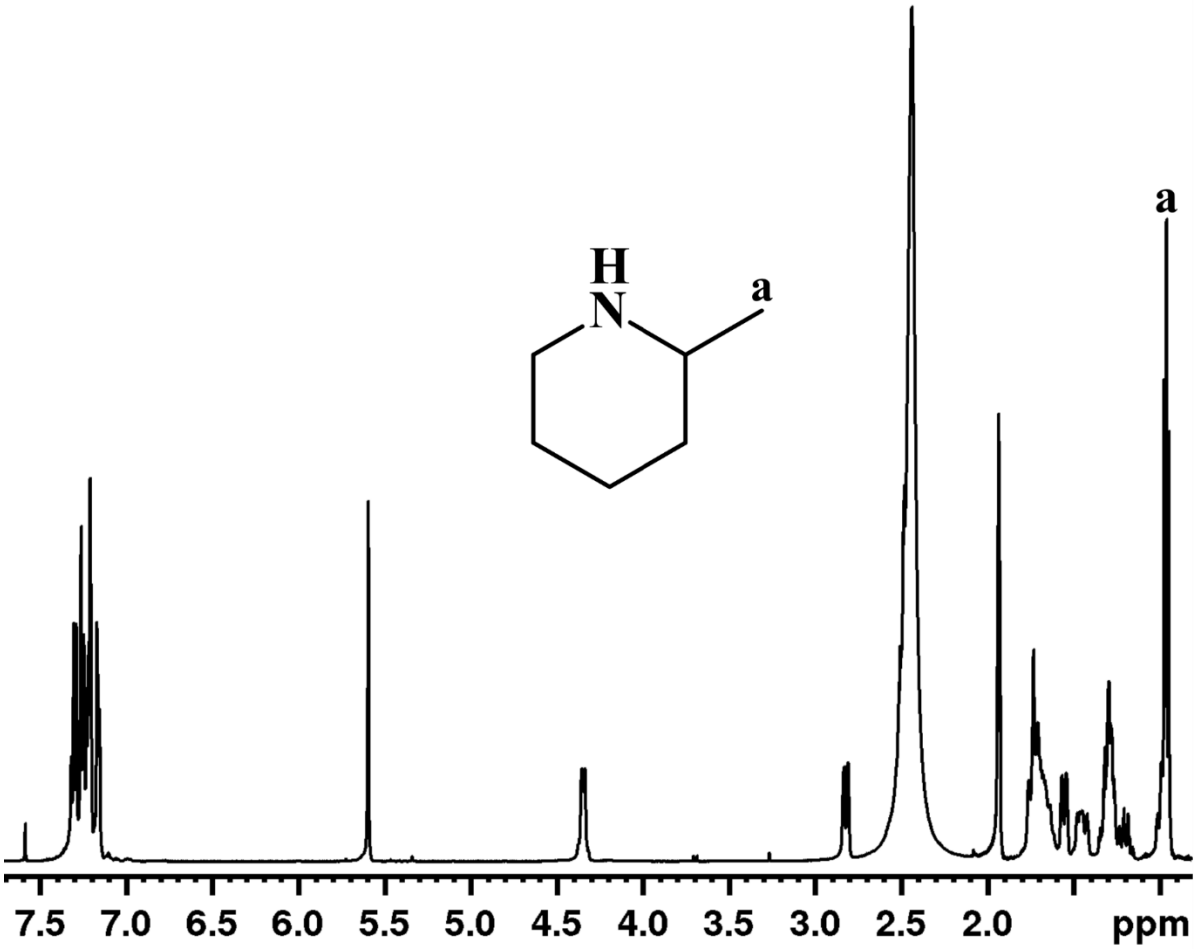
500MHz ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine and (*S*)-CBHA-DPA (1:2) in toluene-d_8(C_7D_8)



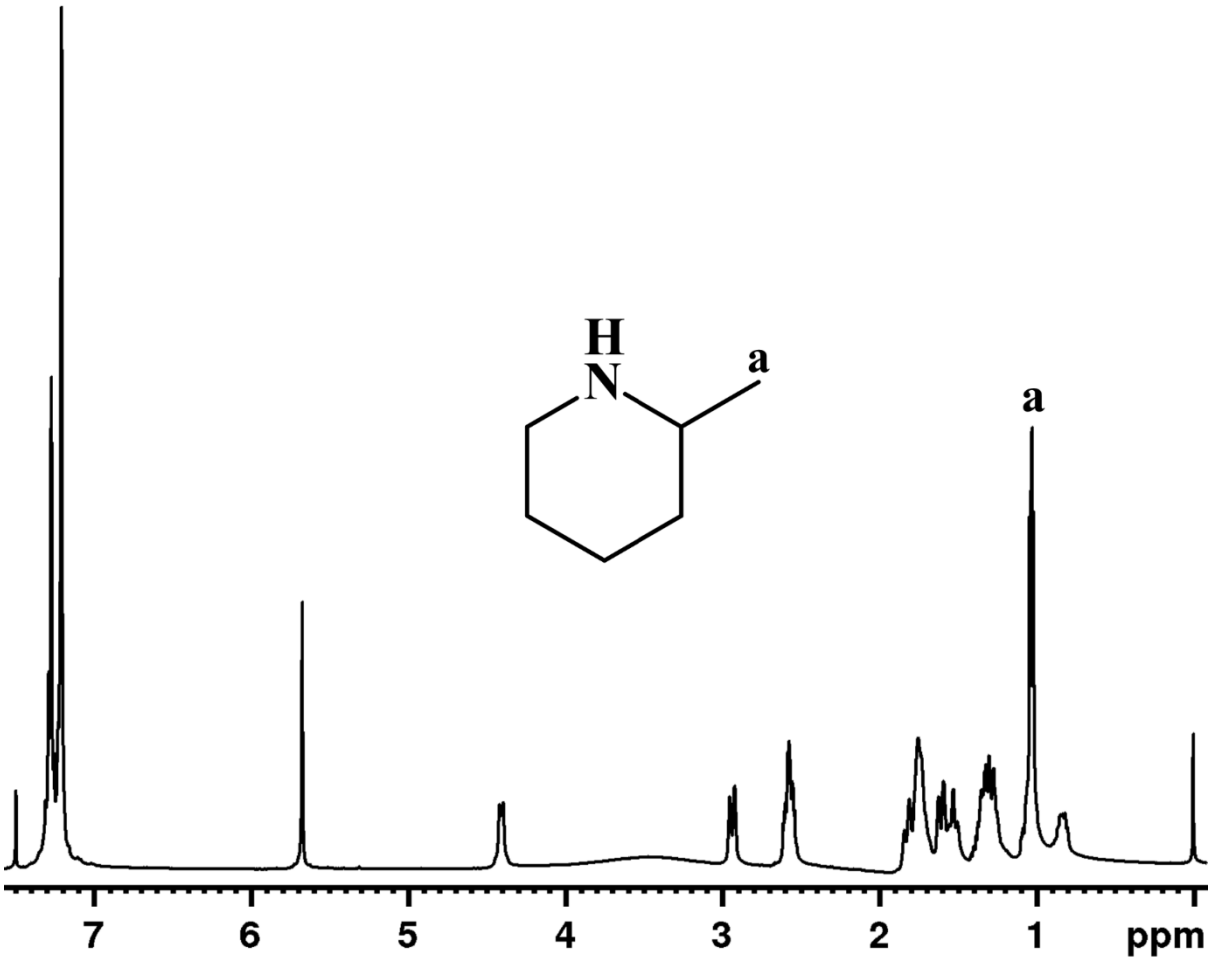
500MHz ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine and (*S*)-CBHA-DPA (1:2) in methylenechloride-d_2(CD_2Cl_2)



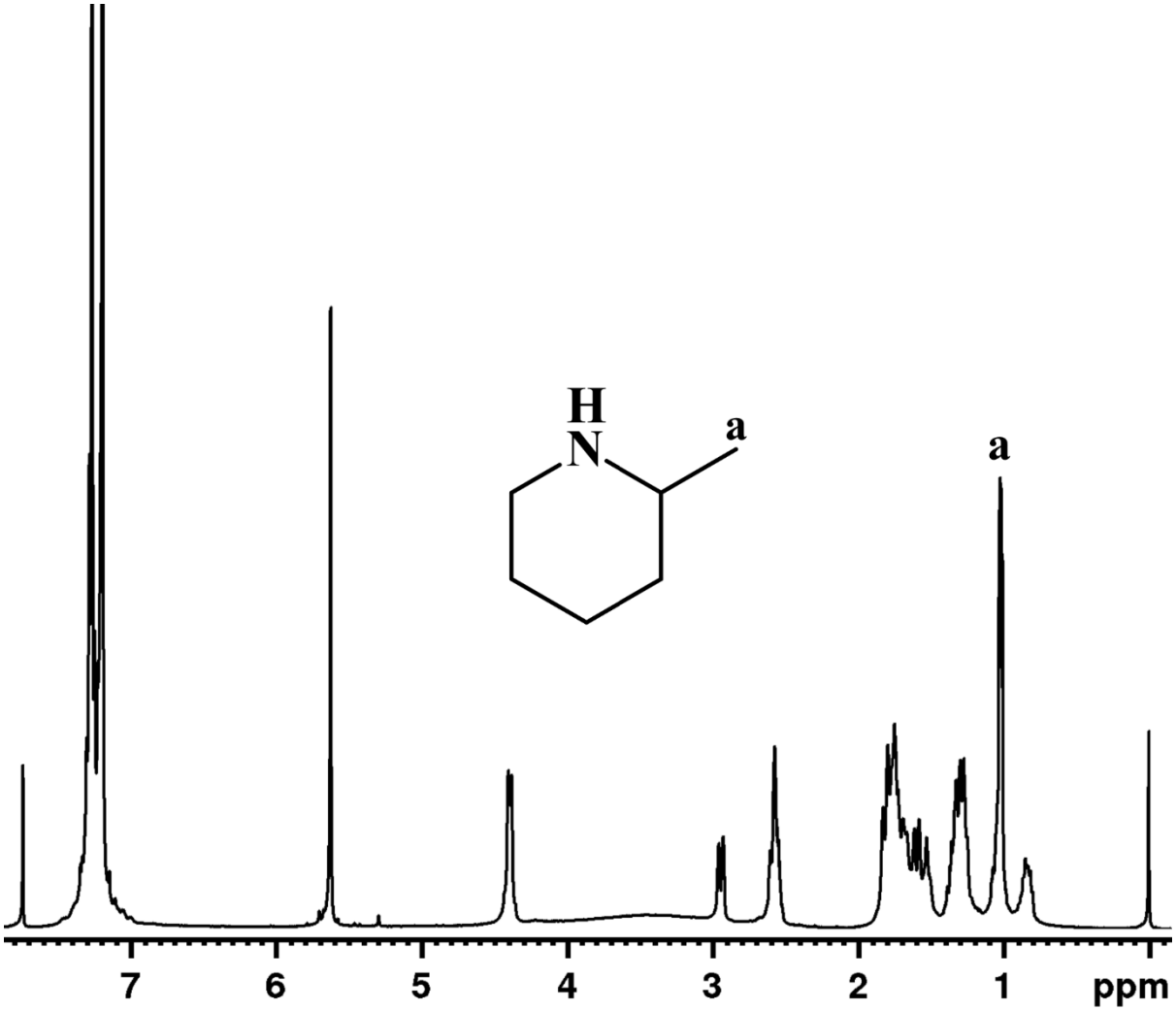
500MHz ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine and (*S*)-CBHA-DPA (1:2) in acetonitrile-d_3 (C_2D_3N)



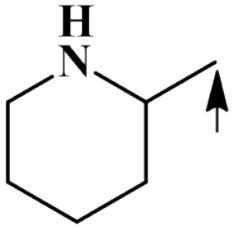
400MHz ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine and (*S*)-CBHA-DPA (1:2) in 10% DMSO in $CDCl_3$



400MHz ^{1}H-NMR spectrum of (*R/S*)-2-methylpiperidine and (*S*)-CBHA-DPA (1:2) in 20% DMSO in $CDCl_3$

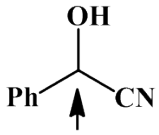
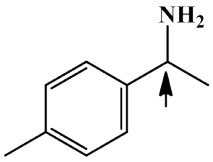
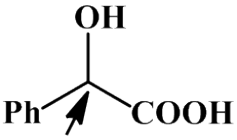
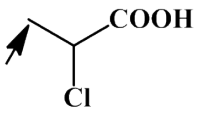
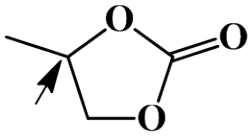
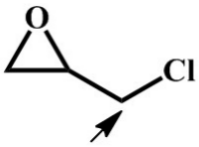


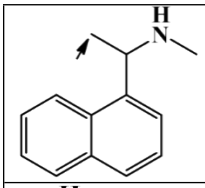
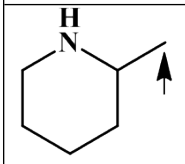
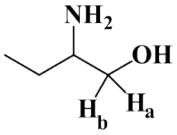
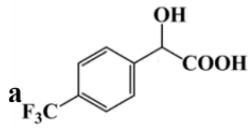
Chemical shift difference for the selected proton of (*R/S)*-2-methylpiperidine with (*S*)-CBHA-DPA (1:2) in different solvents



S.No	Solvent	$\Delta\delta^{R/S}$ (ppm)
1	$CDCl_3$	0.05
2	C_6D_6	0.05
3	TOLUENE-d_8	0.05
4	CD_2Cl_2	0.04
5	CD_3CN	0.01
6	10% DMSO in $CDCl_3$	0.01
7	20% DMSO in $CDCl_3$	0.01

Comparing the present CA with other CAs in the literature

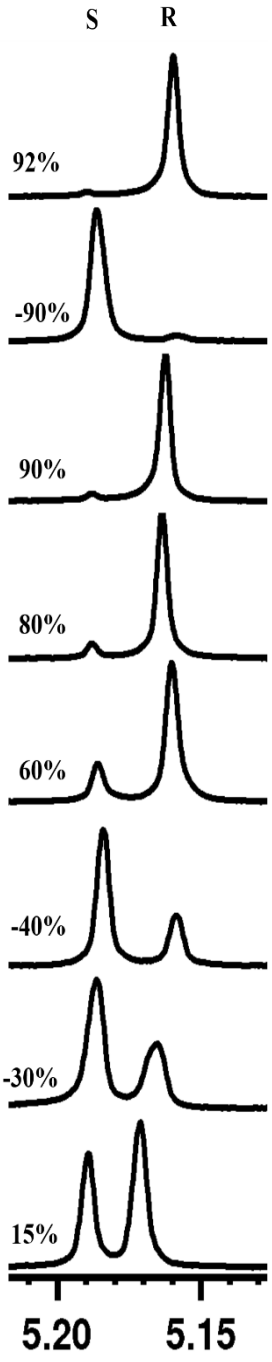
	**1) 0.3** 2) 0.08	1) Present method 2) a) L. S. Moon, R. S. Jolly, Y. Kasetti and P. V Bharatam, *Chem. Commun. (Camb).*, 2009, 1067; b) L. S. Moon, M. Pal, Y. Kasetti, P. V Bharatam and R. S. Jolly, *J. Org. Chem.*, 2010, **75**, 5487.
	**1) 0.07** 2) 0.05 3) 0.01	1) Present method 2) C. F. Dignam, C. J. Richards, J. J. Zopf, L. S. Wacker and T. J. Wenzel, *Org. Lett.*, 2005, **7**, 1773 3) A. E. Lovely and T. J. Wenzel, *Org. Lett.*, 2006, **8**, 2823.
	**1) 0.04** 2) 0.021 3) 0.02	1) Present method 2) L. S. Moon, R. S. Jolly, Y. Kasetti and P. V Bharatam, *Chem. Commun. (Camb).*, 2009, 1067 3) T. P. Quinn, P. D. Atwood, J. M. Tanski, T. F. Moore and J. F. Folmer-Andersen, *J. Org. Chem.*, 2011, **76**, 10020.
	**1) 0.05** 2) 0.024	1) Present method 2) L. S. Moon, R. S. Jolly, Y. Kasetti and P. V Bharatam, *Chem. Commun. (Camb).*, 2009, 1067.
	**1) 0.01** 2) 0.01	1) Present method 2) Couffin, O. Thillaye du Boullay, M. Vedrenne, C. Navarro, B. Martin-Vaca and D. Bourissou, *Chem. Commun. (Camb).*, 2014, **50**, 5997.
	**1) 0.15** 2) 0.065	1) Present method 2) Couffin, O. Thillaye du Boullay, M. Vedrenne, C. Navarro, B. Martin-Vaca and D. Bourissou, *Chem. Commun. (Camb).*, 2014, **50**, 5997.

	**1) 0.03** 2) 0.02	1) Present method 2) A. E. Lovely and T. J. Wenzel, *Org. Lett.*, 2006, **8**, 2823.
	**1) 0.06** 2) 0.05	1)Present method 2) A. E. Lovely and Thomas J. Wenzel,*J. Org. Chem.* 2006, *71*, 9178.
	**1) a 0.04,** **b 0.09** 2) a 0.01 b 0.05	1) Present method 2) A. E. Lovely and T. J. Wenzel, *J. Org. Chem.*, 2006, **71**, 9178.
	**19F** **[a]1) 0.03** 2) 0.033 3) 0.03	1) Present method 2) N. Jain, M. B. Mandal and A. V. Bedekar, *Tetrahedron*, 2014, **70**, 4343. 3) S. R. Chaudhari and N. Suryaprakash, *J. Org. Chem.*, 2012, **77**, 648.

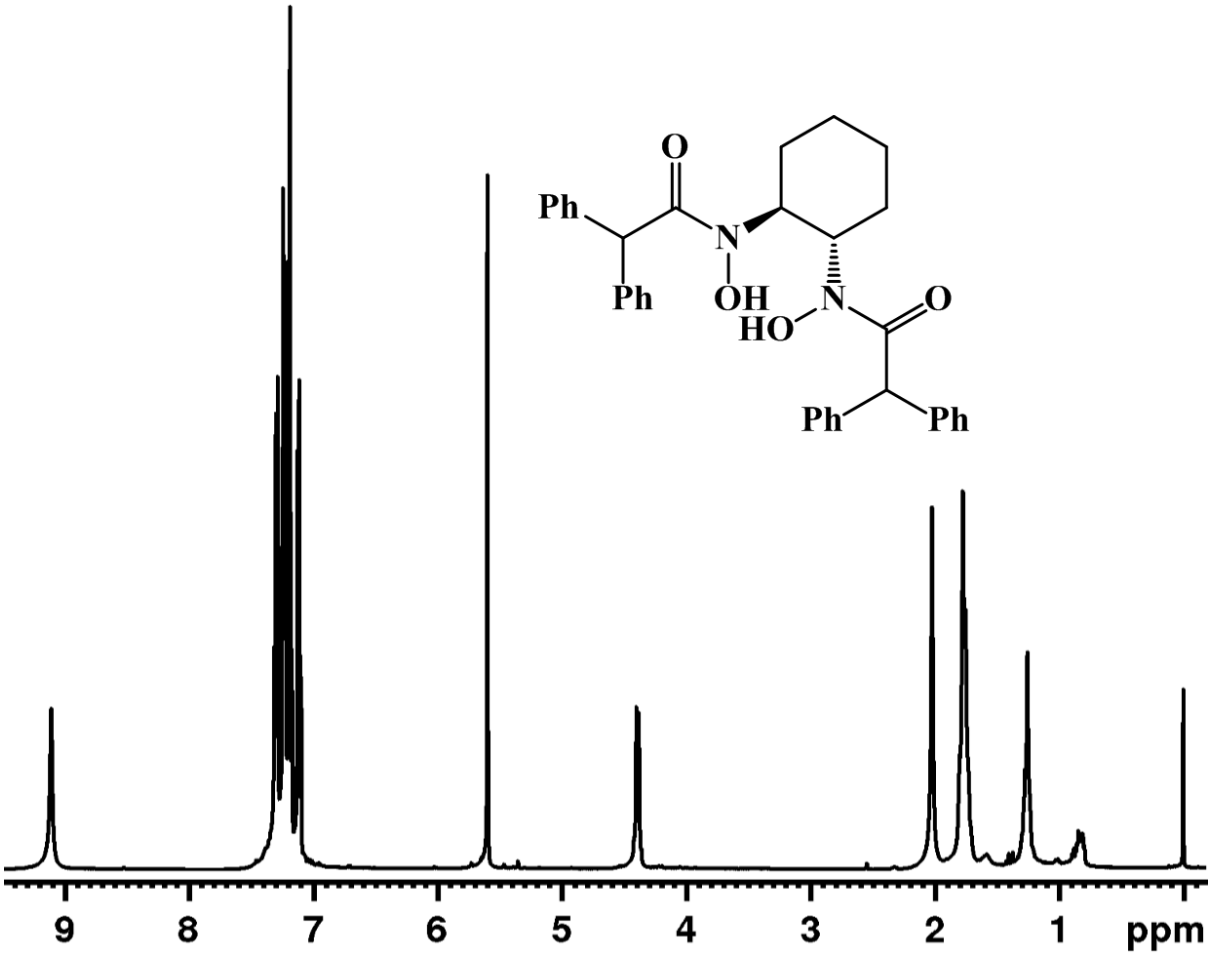
The experimentally determined and laboratory prepared scalemicratios of (*R/S*) – Mandelic acid and (*S*)-CBHA-DPA. Alpha proton was chosen to measure*ee*.

Entry	Integration I_R:I_S	Gravimetrically prepared excess of R enantiomer	$ee\% = \frac{I_R - I_S}{I_R + I_S} \times 100$ experimentally measured enantiomeric excess
1	1.000:0.043	92	91.7
2	1.000:0.056	90	89.9
3	1.000:9.048	80	80.0
4	1.000:0.731	15	15.3
5	1.000:2.383	-40	-40.2
6	1.000:1.853	-30	-29.9
7	1.000:15.533	-90	-89.8
8	1.000:0.251	60	59.8

400 MHz ^{1}H-NMR spectra of selected regions of different scalemic ratios of *R*–mandelic acid and *S*-mandelic acid in $CDCl_3$



500MHz ^{1}H-NMR spectrum of (*S*)-CBHA-DPA in $CDCl_3$



Pure shift NMR experimental details:

Pure shift NMR experiment: The pure shift spectroscopy suppresses the effects of homonuclear coupling, allowing ^{1}H spectra to be produced that contain chemical shifts only, with no multiplet structure, a major improvement in the resolution. The pure shift experiment was performed on 500 MHz Bruker spectrometer by using "push1dzs" pulse program which is available in the public domain of the Manchester NMR methodology group website (http://nmr.chemistry.manchester.ac.uk). This pulse program produces a pseudo 2D experiment where the delay between excitation and detection is incremented stepwise. The refocusing step was carried out using rsnob shaped pulse combined with slice selection gradient strength of 0.7 to 0.9 G cm^{-1}. Each of the 32 increments in t_1 was acquired with 8 scans with a recycle delay of 2 s between two successive fids. The total time domain points in t_2 dimension are 2K. Data was processed with the AU program named pshift present at the same website (http://nmr.chemistry.manchester.ac.uk). The AU program converts the raw data to pure shift FID. The spectra were recorded in CDCl3 at 298K.