Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPORTING INFORMATION

p -TsOH enables 2'-amino-[1, 1'-binaphthalene]-2-ol as a Chiral Solvating Agent

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S48: 400 MHz^{1}H-NMR spectra of (*R*) -Mandelic acid and P-Toluene sulphonic acid in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN

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S52: 400 MHz ^{1}H-NMR spectra of (*R*)-4-Chloromandelic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN

S53: 400 MHz ^{1}H-NMR spectra of (*L*) -Lactic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN

S54: 400 MHz ^{1}H-NMR spectra of (*S*) -2-Hydroxy-3-methyl butyric acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN

S55: 400 MHz ^{1}H-NMR spectra of (*S*) -2-Hydroxy-3, 3-dimethyl butyric acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN

S56: 400 MHz ^{1}H-NMR spectra of (*R*) -2-Chloro mandelic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN

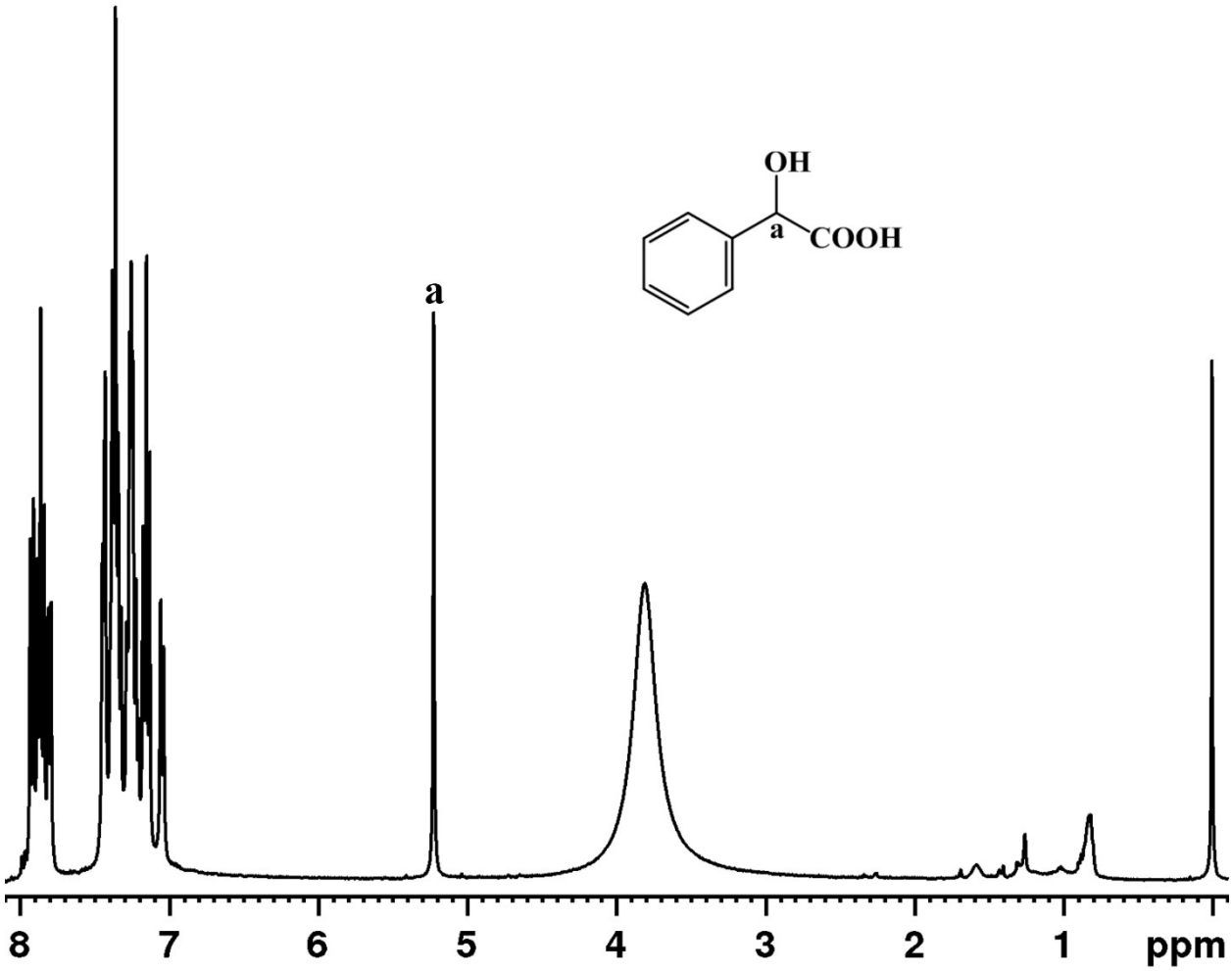
Experimental Details

The commercially available (*R*) - 2'-amino-[1, 1'-binaphthalen]-2-ol ((*R*)-NOBIN), the molecules 1-18, and chloroform-d were purchased and used as received. The ^{1}H, ^{13}C, TOCSY, COSY and HSQC NMR spectra were recorded on 400 MHz spectrometer and referenced with respect to TMS.

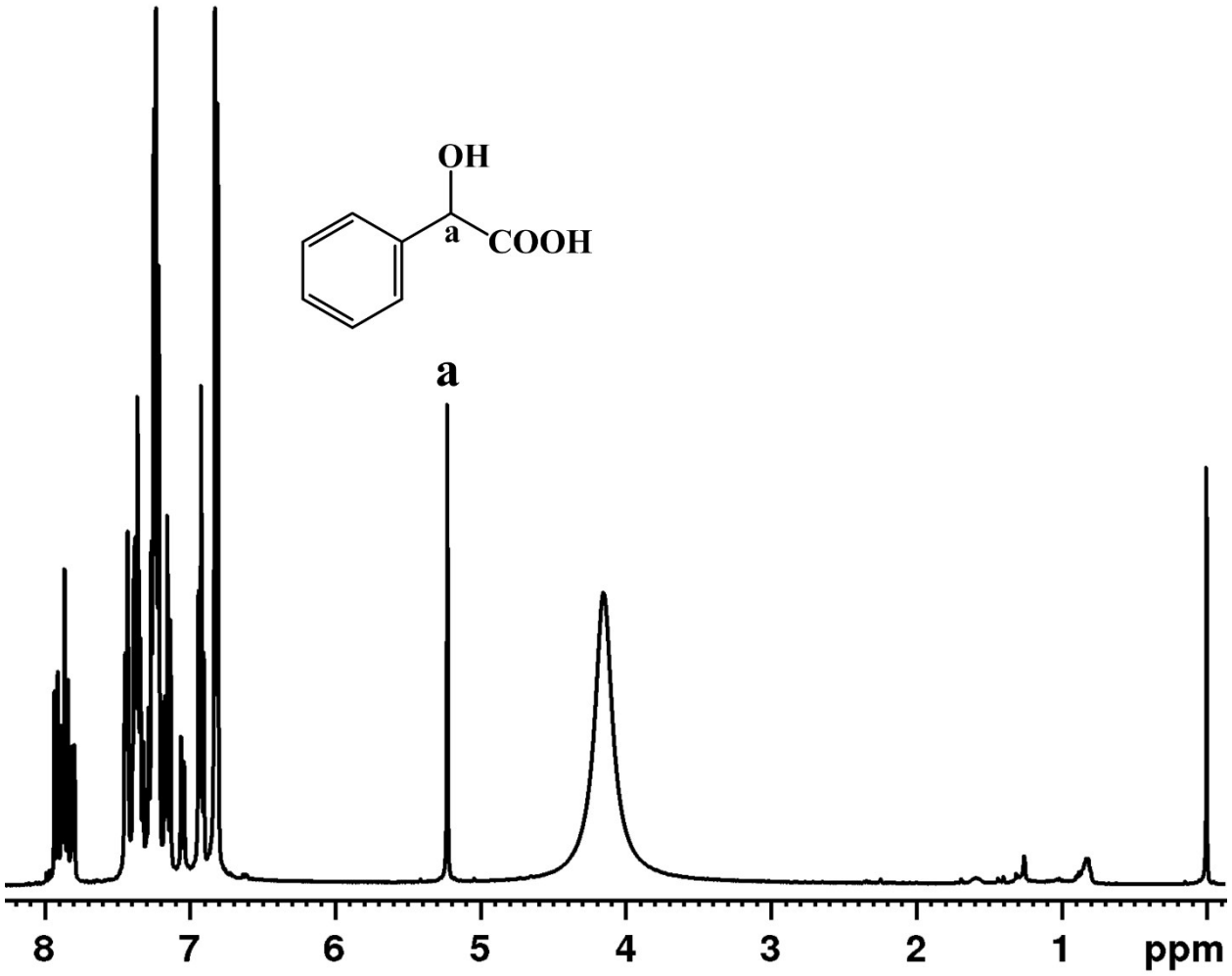
Parameters	TOCSY	COSY	HSQC
Pulseprog	mlevph	cosygpqf	hsqcetgp
Time domain points(TD)	2048 (F2), 416 (F1)	1024 (F2), 256 (F1)	1024 (F2), 256 (F1)
Number of scans (NS)	16	16	16
Number of dummy scans (DS)	16	16	16
FnMODE	States-TPPI	QF	Echo-Antiecho
Mixing time	60ms	…… ….	……..

S1

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

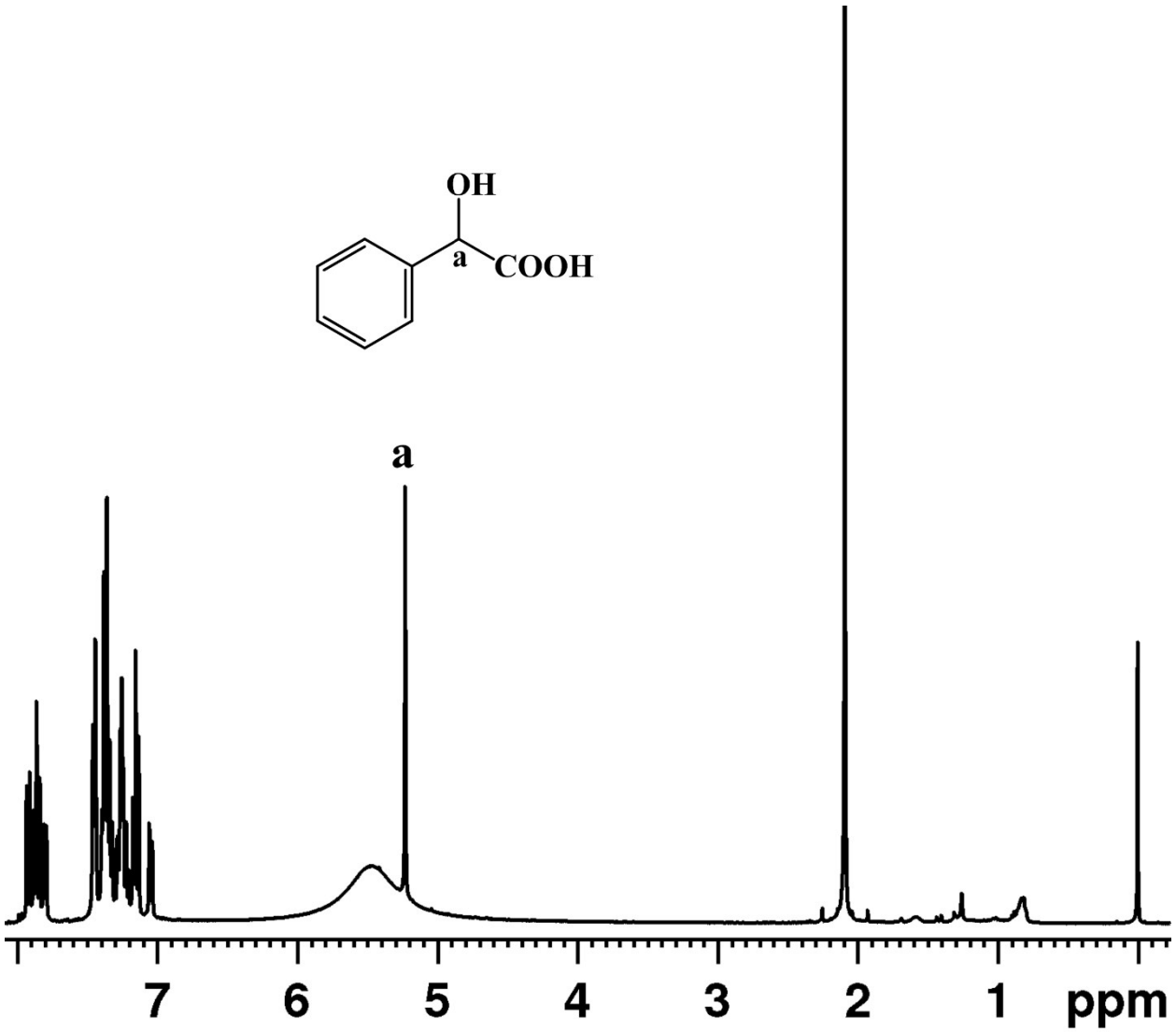


400 MHz ^{1}H-NMR spectrum of (*R/S*)-Mandelic acid, (*R*)-NOBIN and Phenol in $CDCl_3$

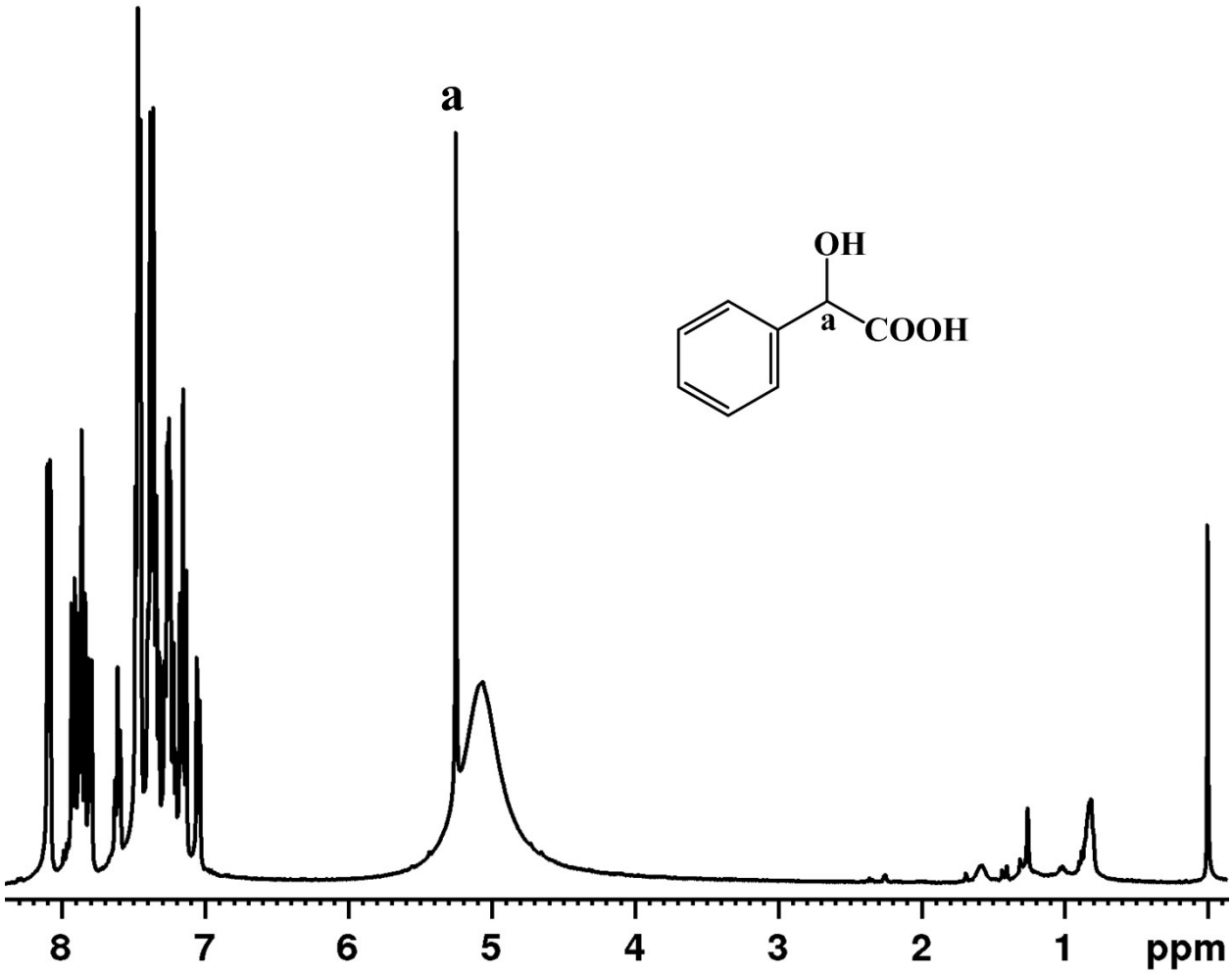


S3

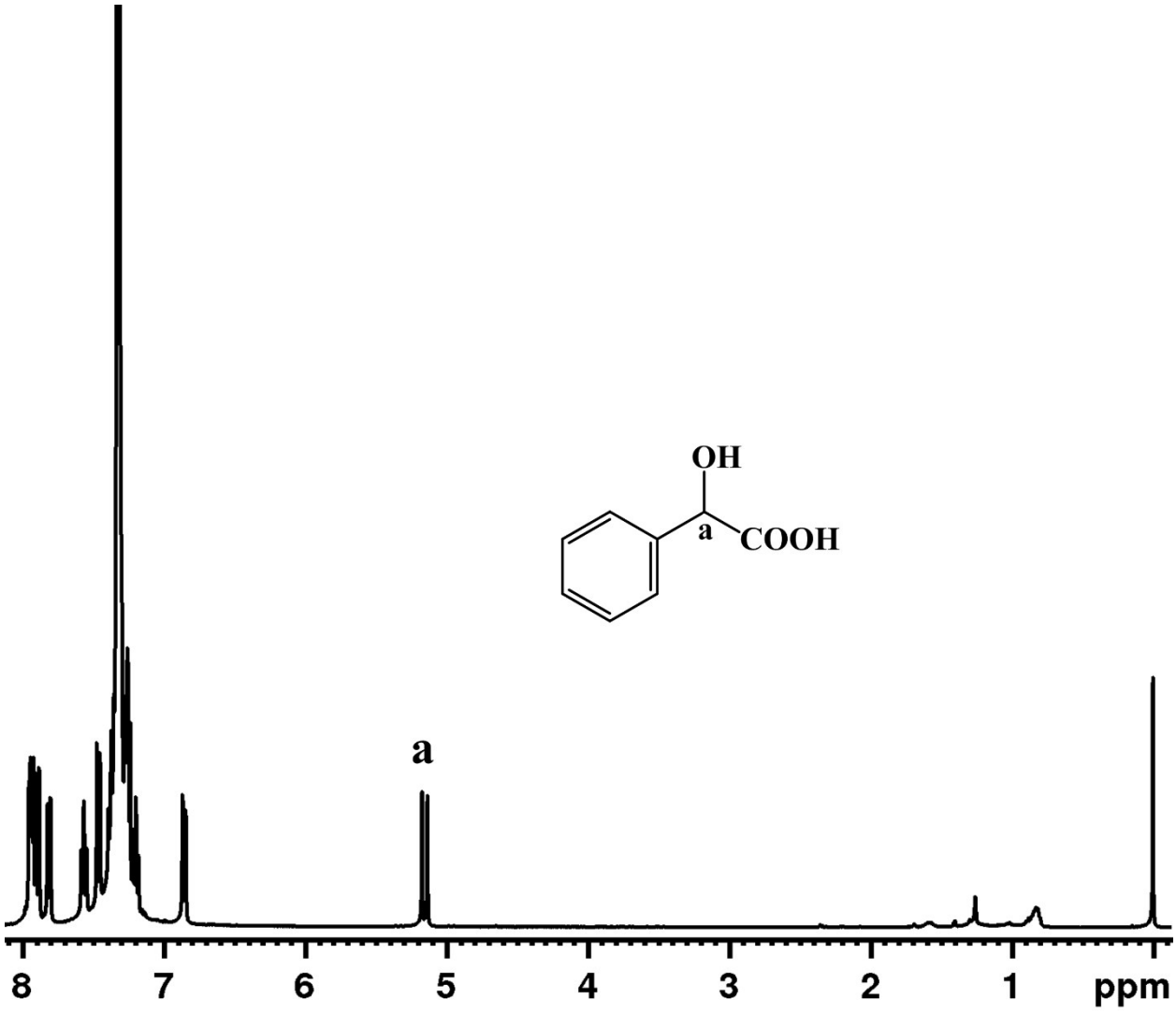
400 MHz ^{1}H-NMR spectrum of (*R/S*)-Mandelic acid, (*R*)-NOBIN and Acetic acid in $CDCl_3$



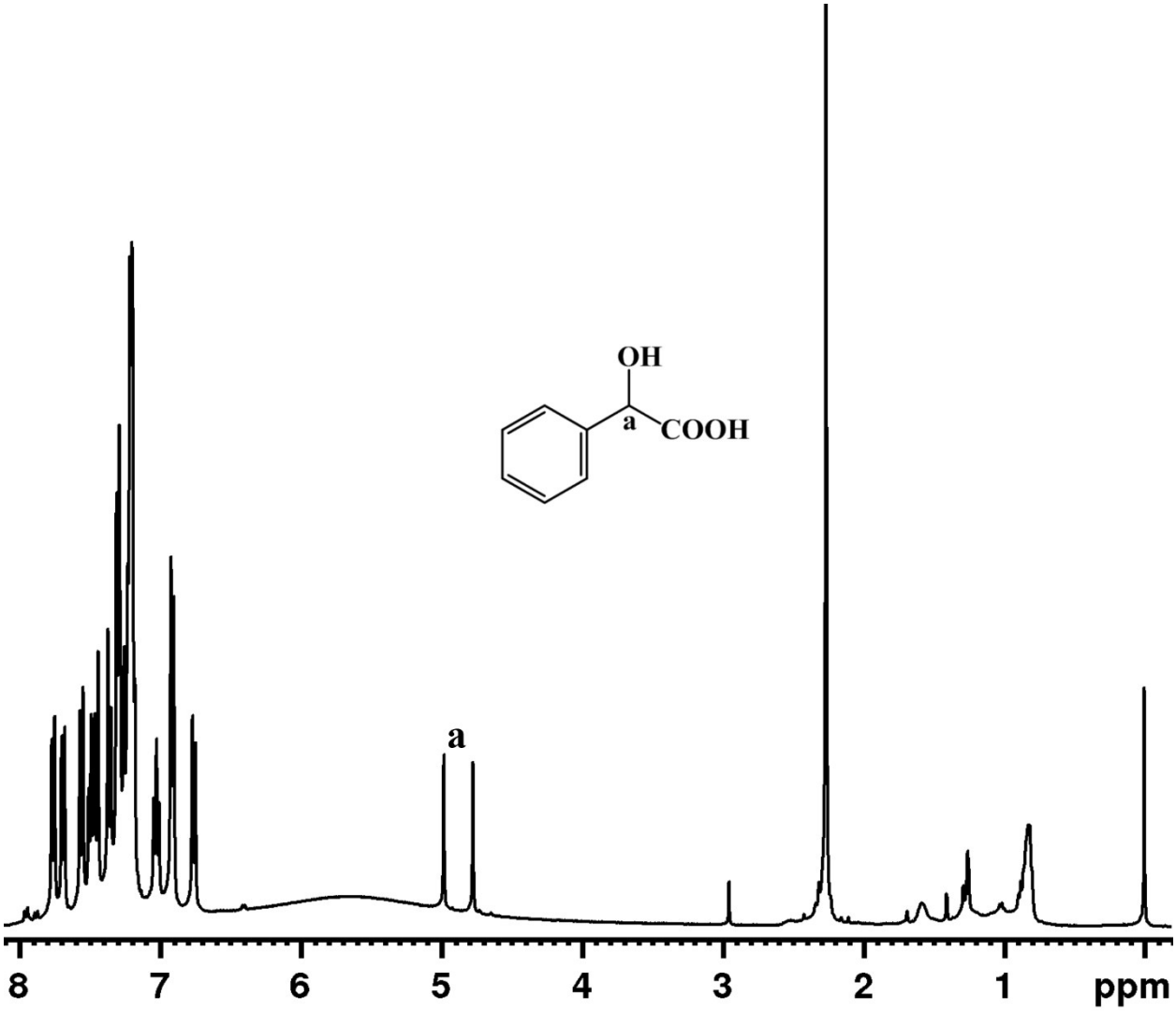
400 MHz ^{1}H-NMR spectrum of (*R/S*)-Mandelic acid, (*R*)-NOBIN and Benzoic acid in $CDCl_3$



400 MHz ^{1}H-NMR spectrum of (*R/S*)-Mandelic acid, (*R*)-NOBIN and Trifluoro acetic acid in $CDCl_3$

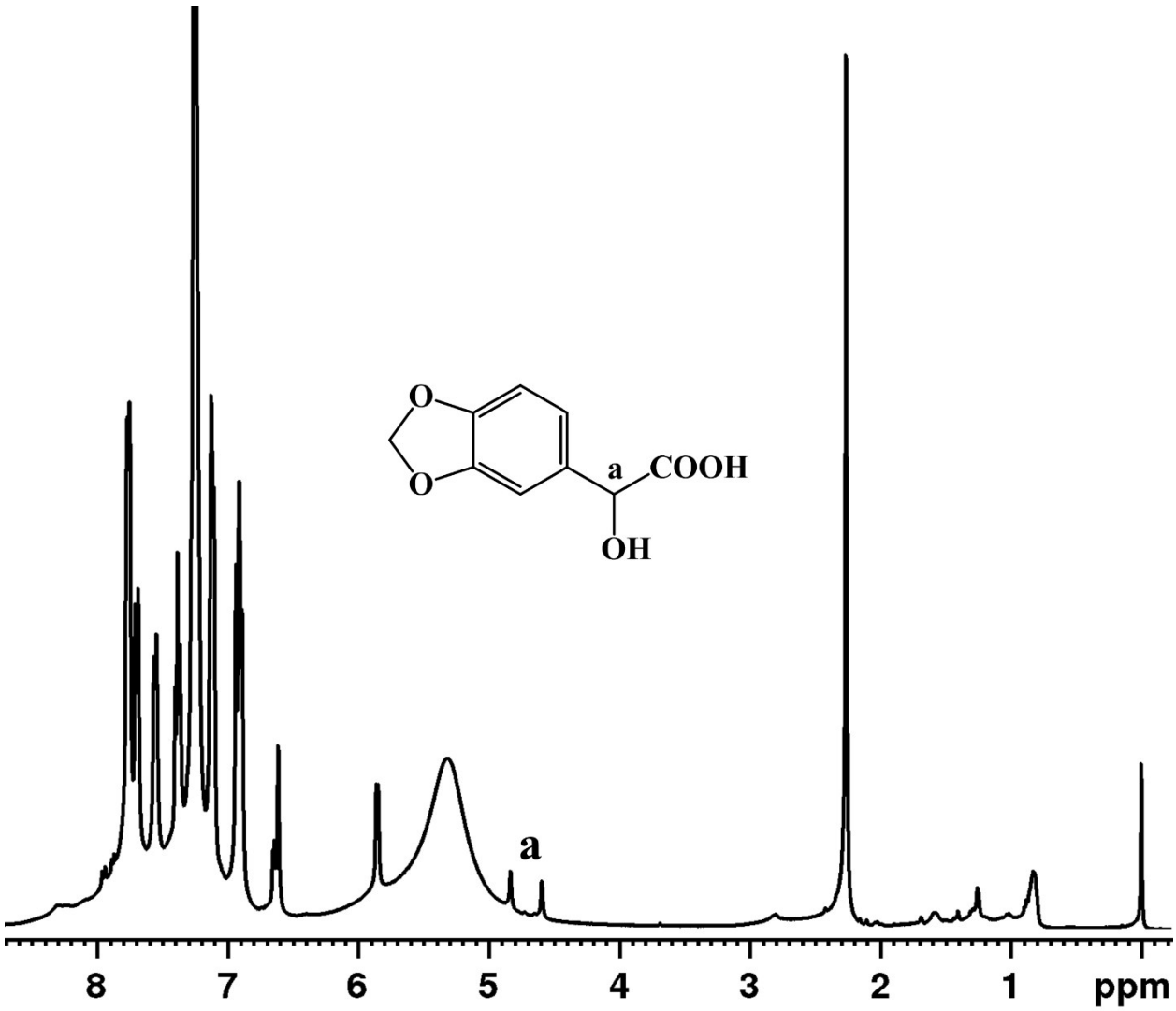


400 MHz ^{1}H-NMR spectrum of (*R/S*)-Mandelic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



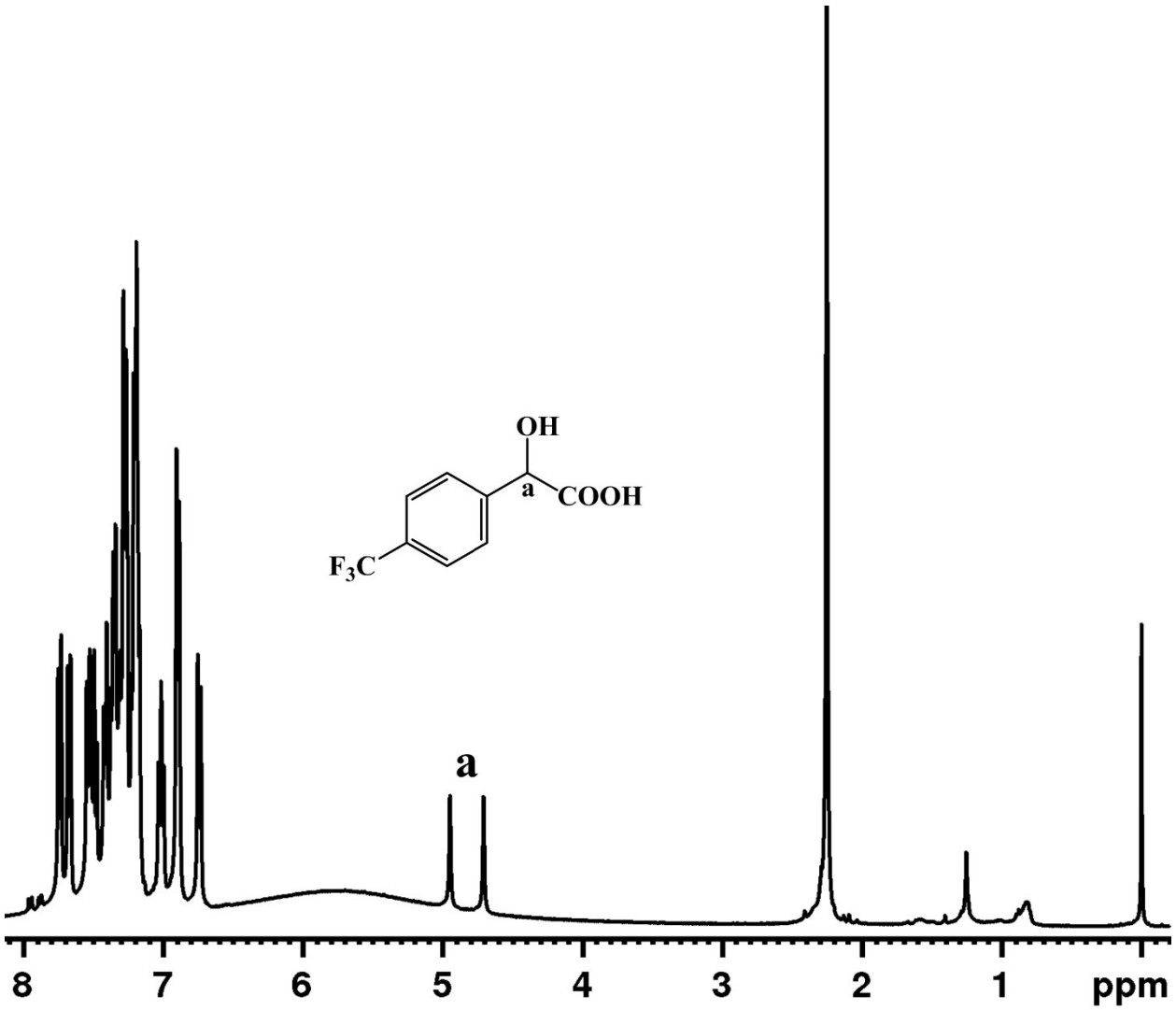
S7

400 MHz ^{1}H-NMR spectrum of (*R/S*)-3, 4-(Methylenedioxy) mandelic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



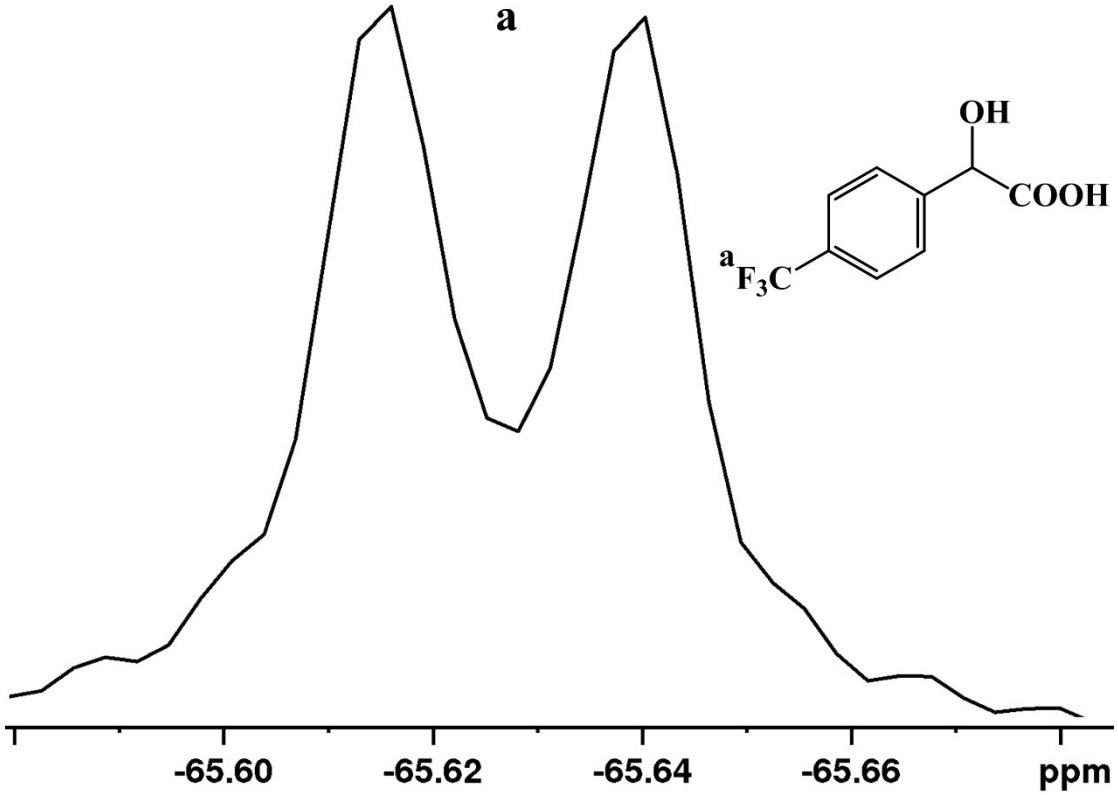
S8

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



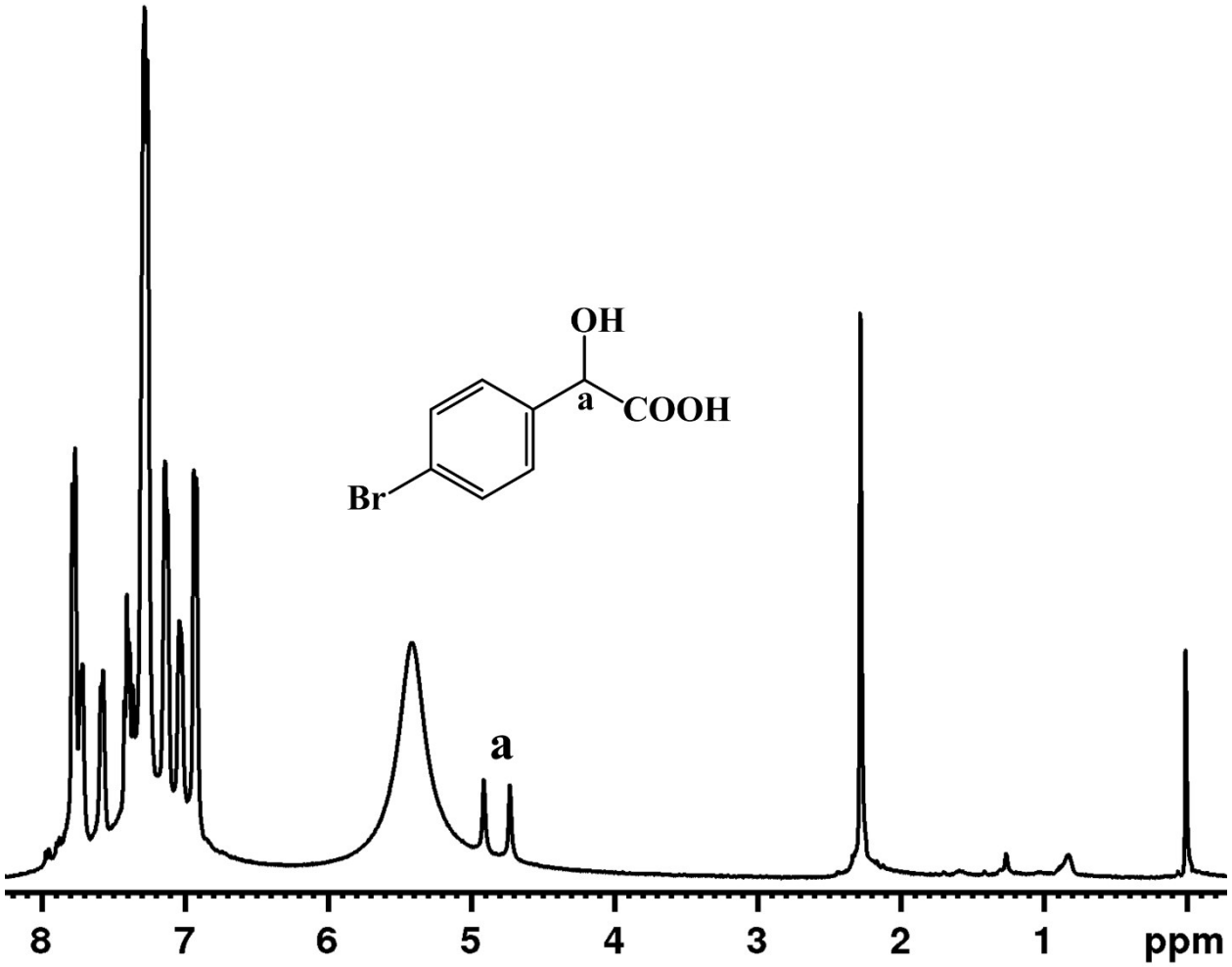
S9

376 MHz ^{19}F-NMR spectrum of (*R/S*)-4-(Trifluoromethyl)mandelic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



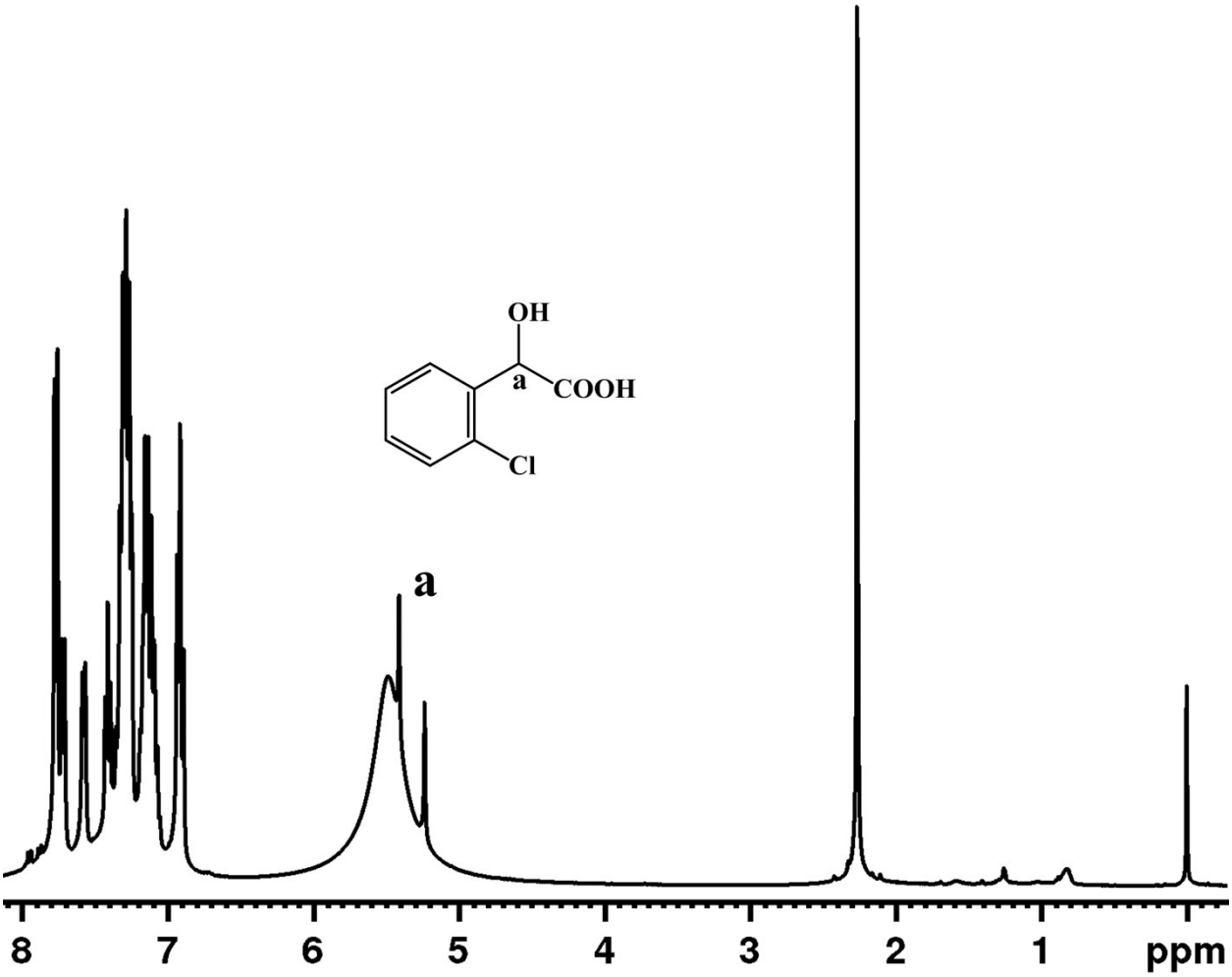
S10

400 MHz ^{1}H-NMR spectrum of (*R/S*)-4-Bromomandelic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



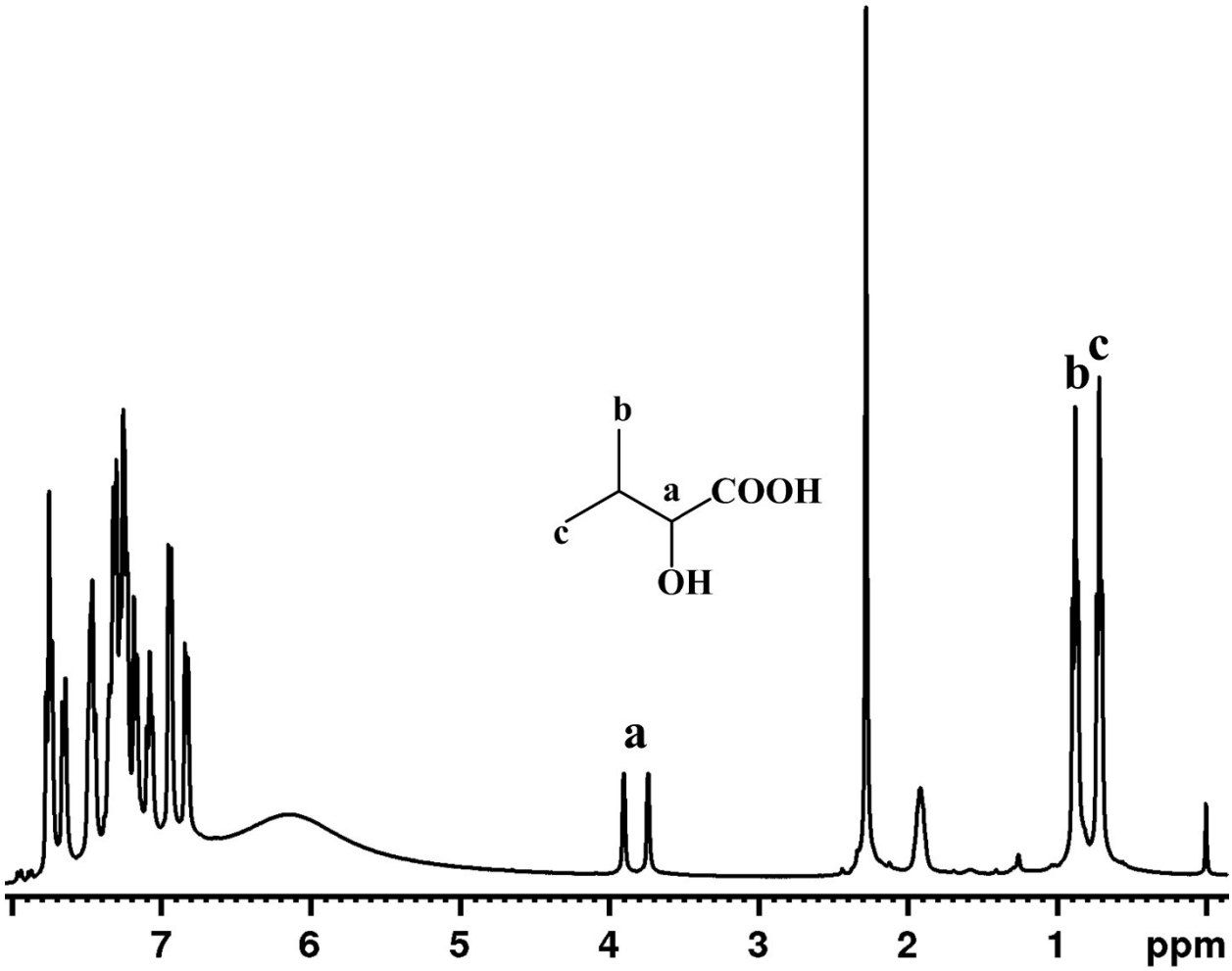
S11

400 MHz ^{1}H-NMR spectrum of (*R/S*) -4-Chloromandelic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



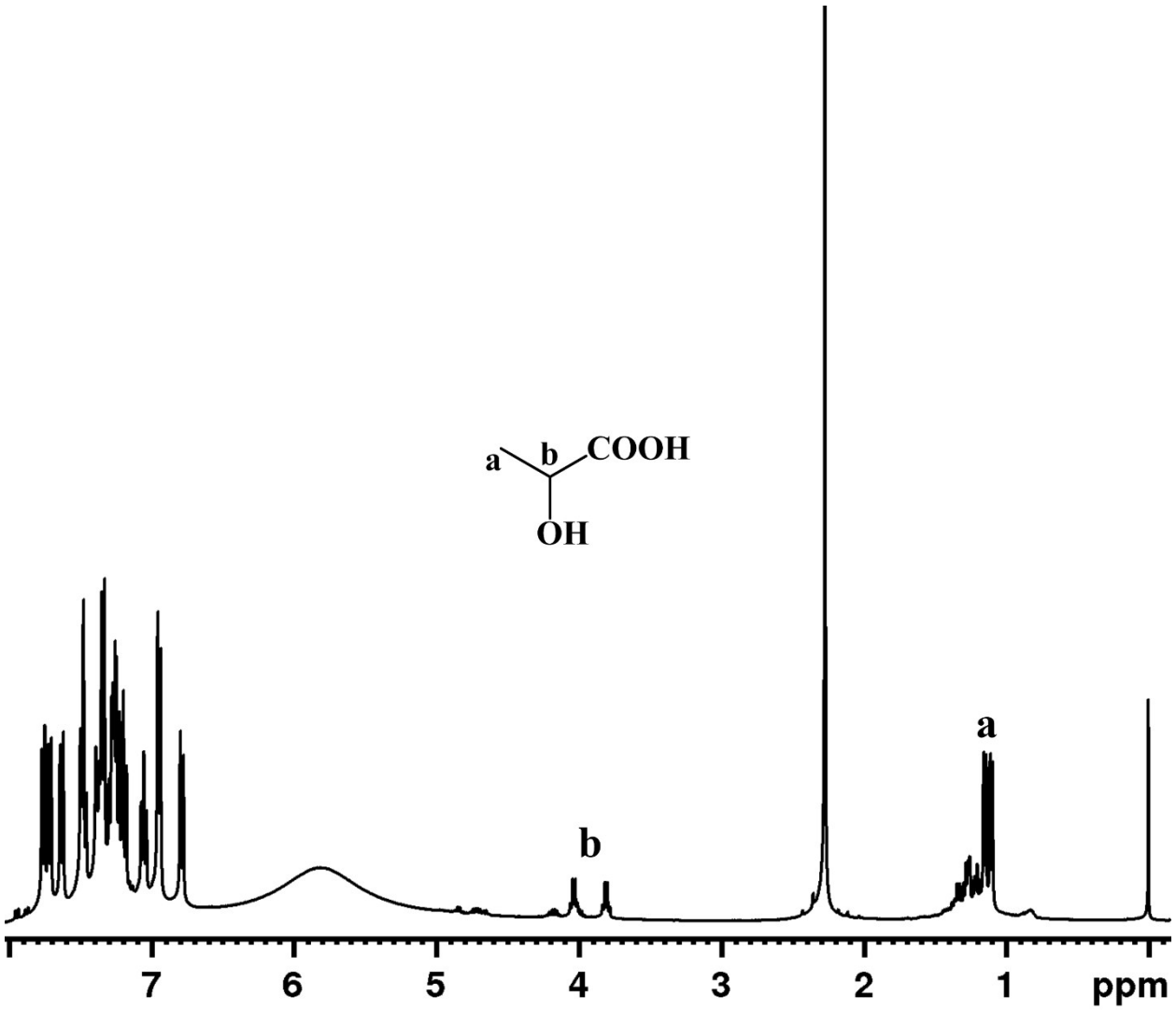
S12

400 MHz ^{1}H-NMR spectrum of (*R/S*)-2-Hydroxy-3-methyl butyric acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$

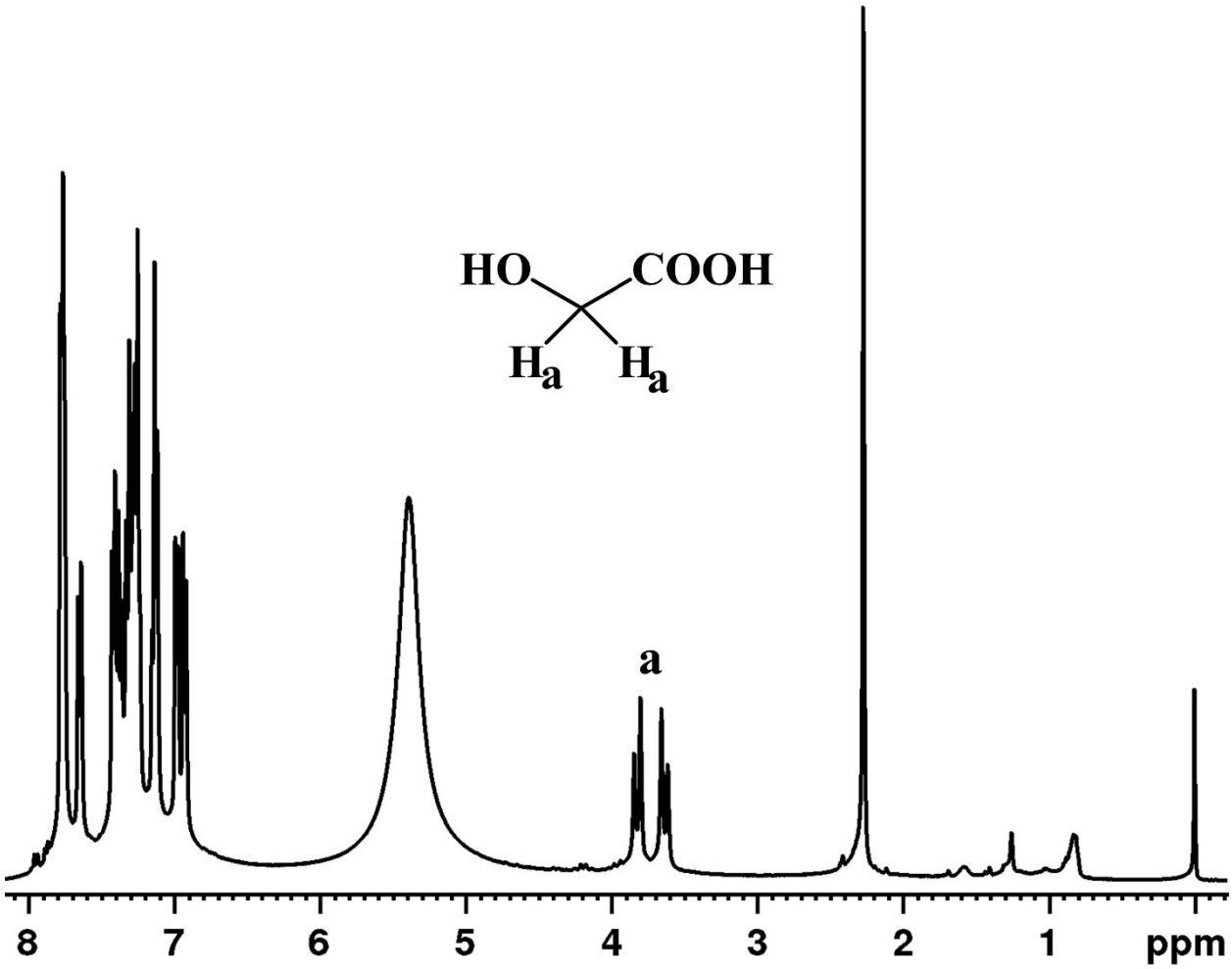


S13

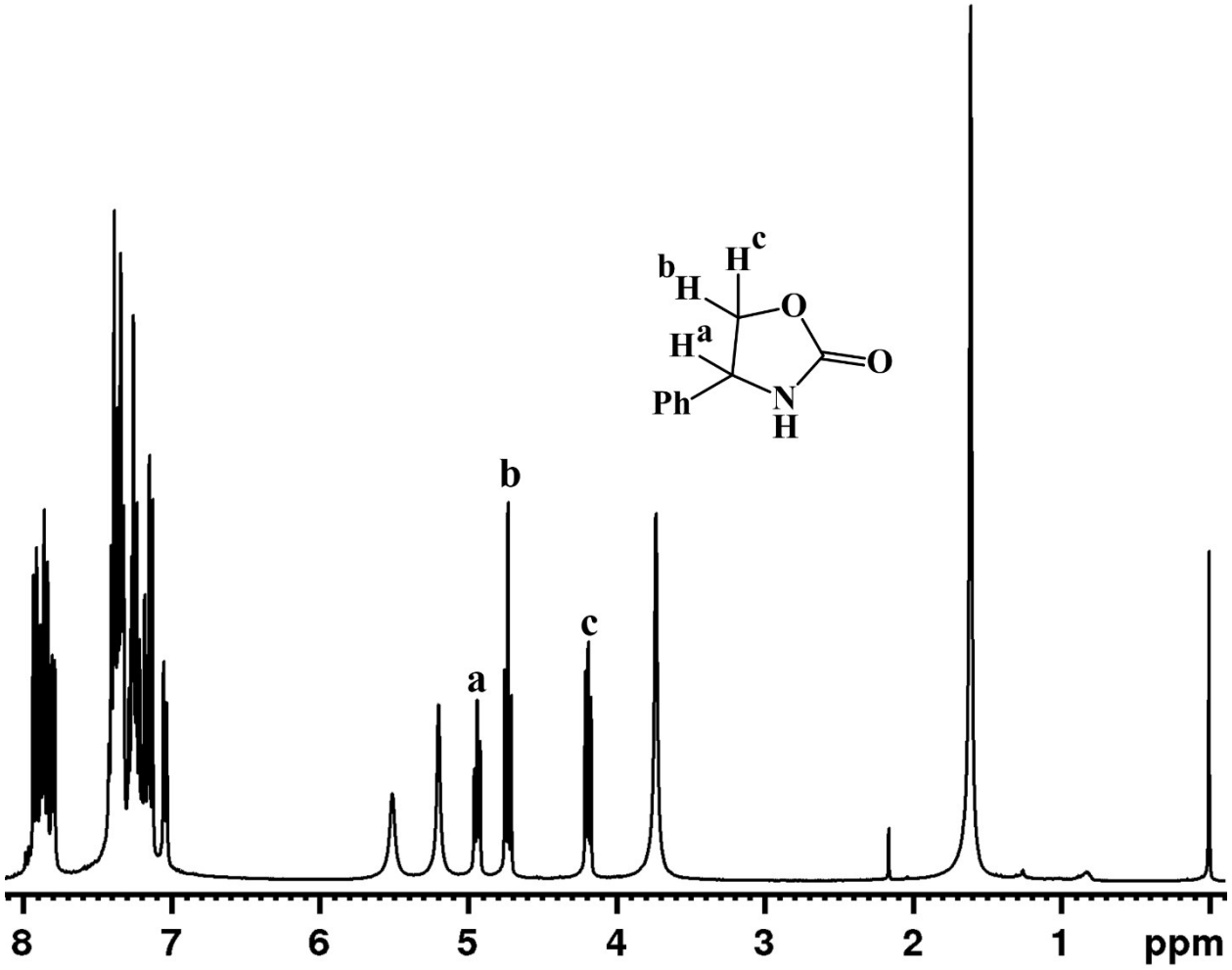
400 MHz ^{1}H-NMR spectrum of (*DL*) –Lactic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



400 MHz ^{1}H-NMR spectrum of Glycolic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$

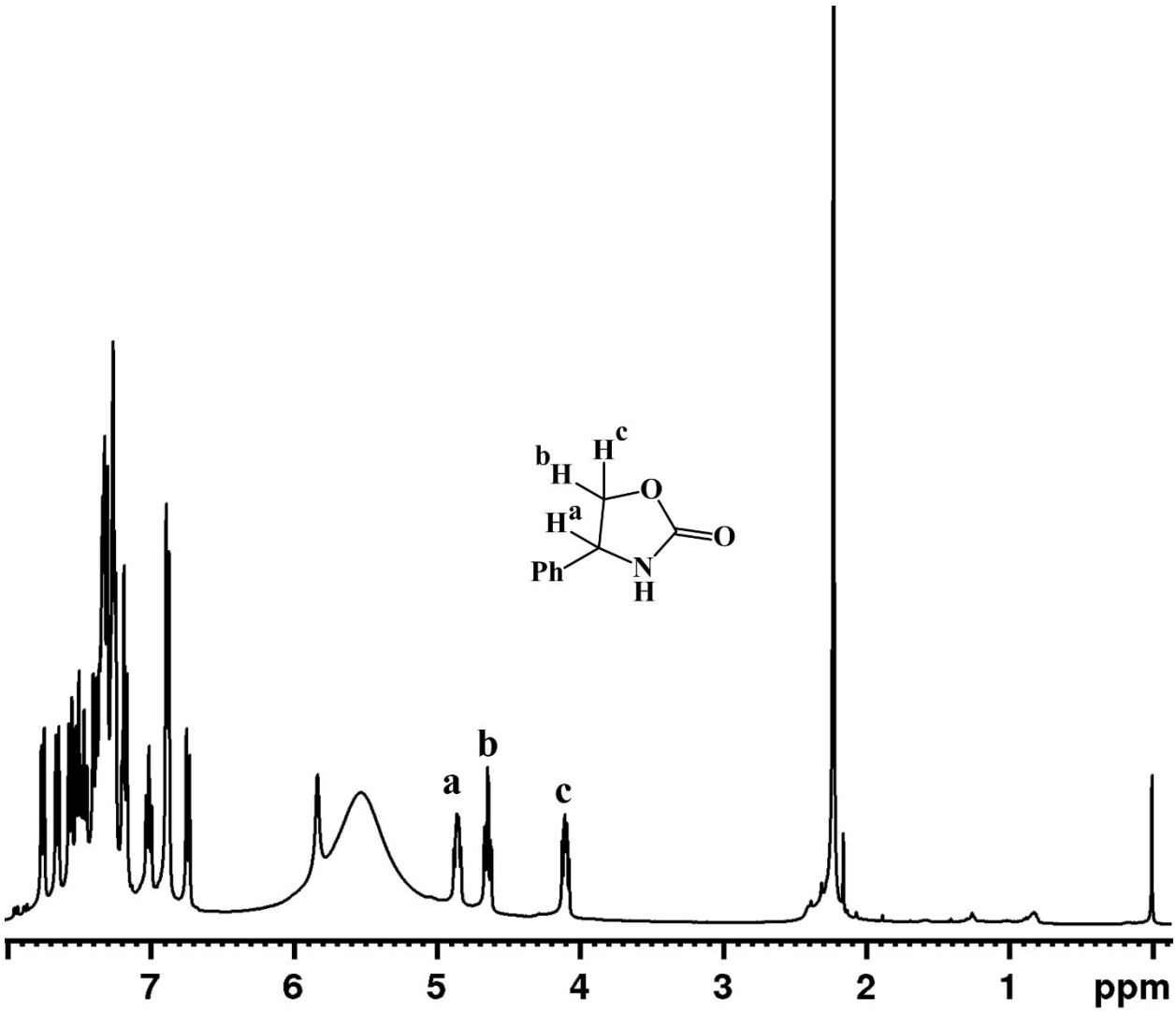


400 MHz ^{1}H-NMR spectrum of (*R/S*) -4-Phenyl-2-oxazolidinone and (*R*)-NOBIN in $CDCl_3$

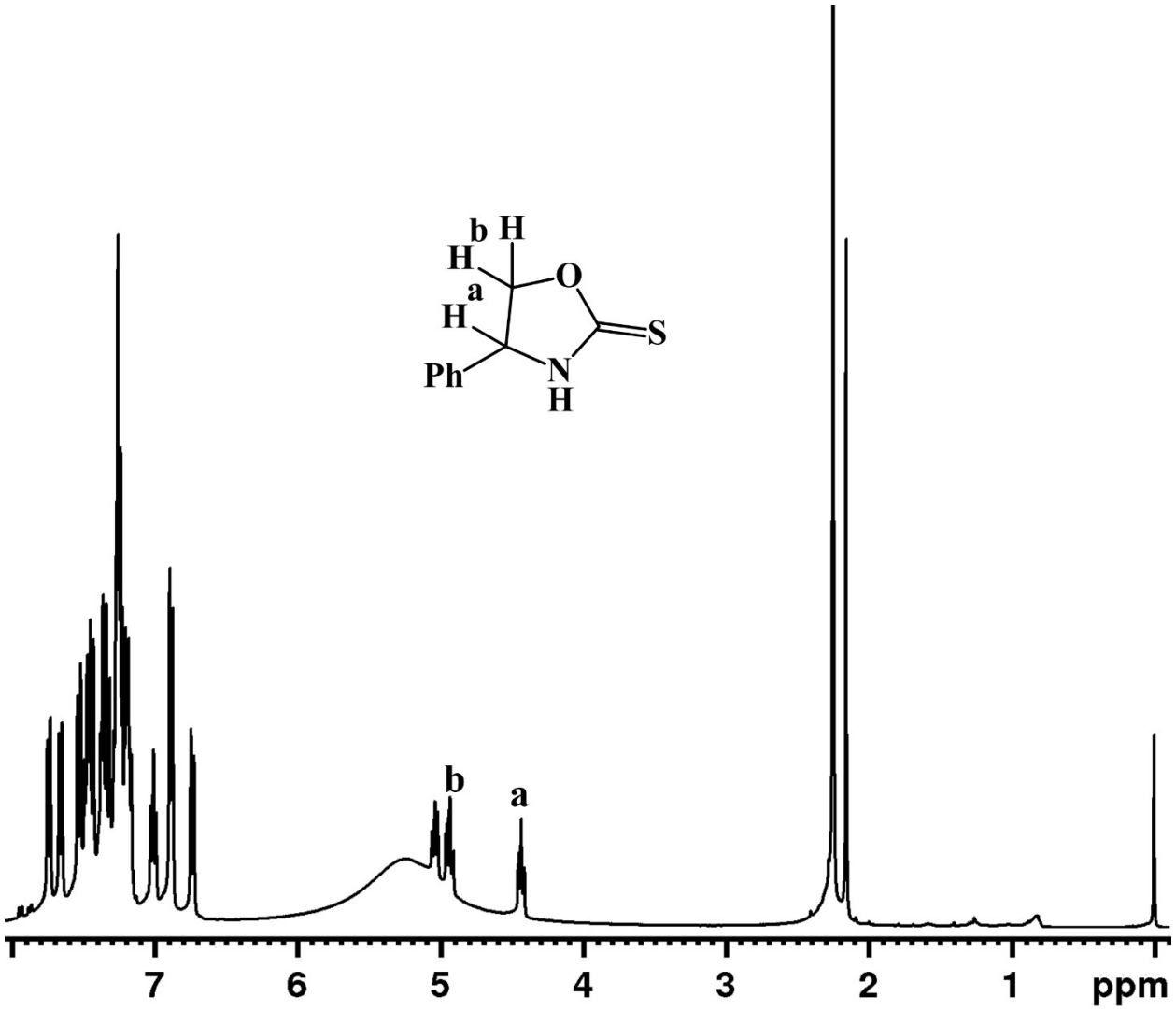


S16

400 MHz ^{1}H-NMR spectrum of (*R/S*)-4-Phenyl-2-oxazolidinone, (*R*)-NOBIN and p-TsOH in $CDCl_3$

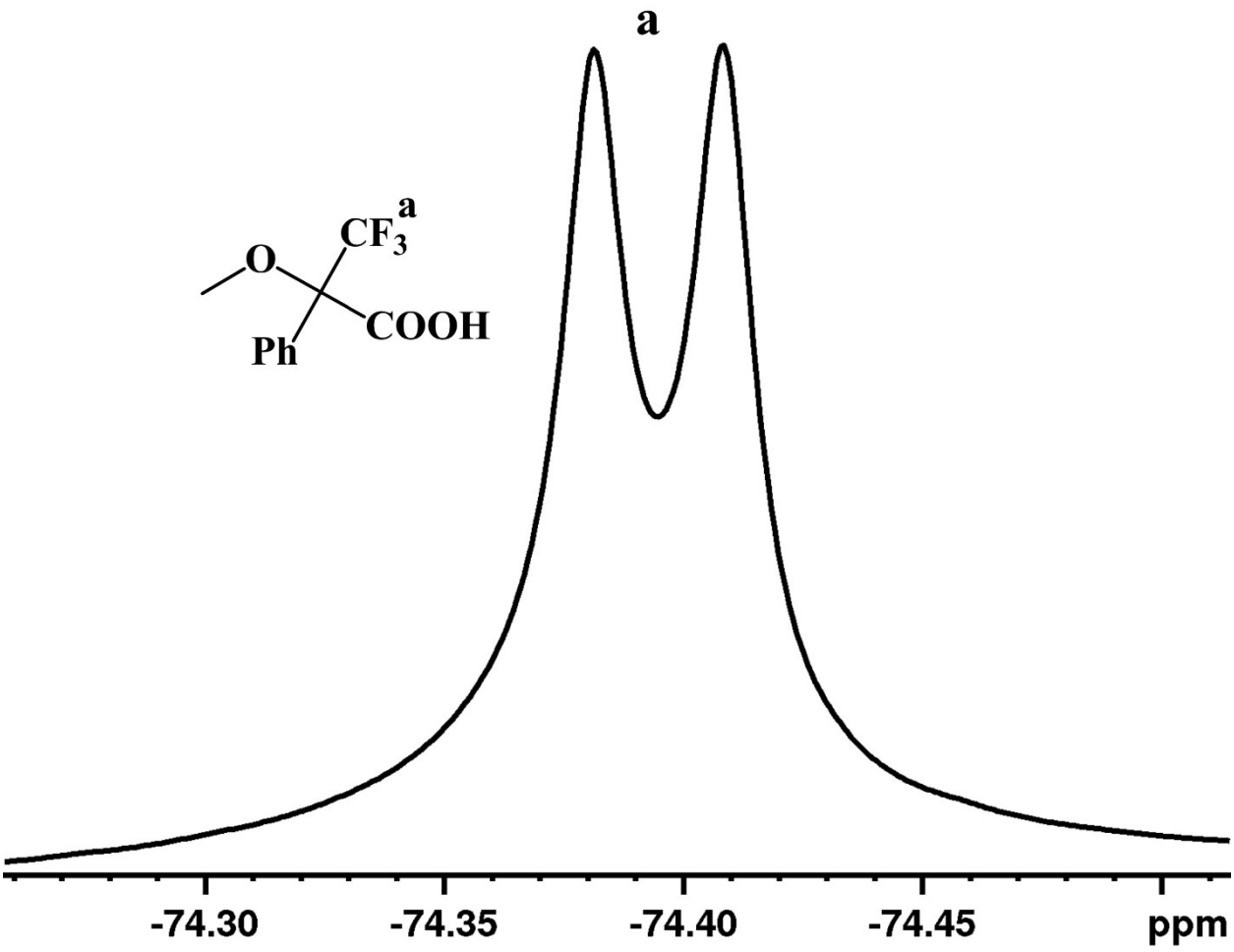


400 MHz ^{1}H-NMR spectrum of (*R/S*)-4-Phenyloxazolidine-2-thione, (*R*)-NOBIN and p-TsOH in $CDCl_3$

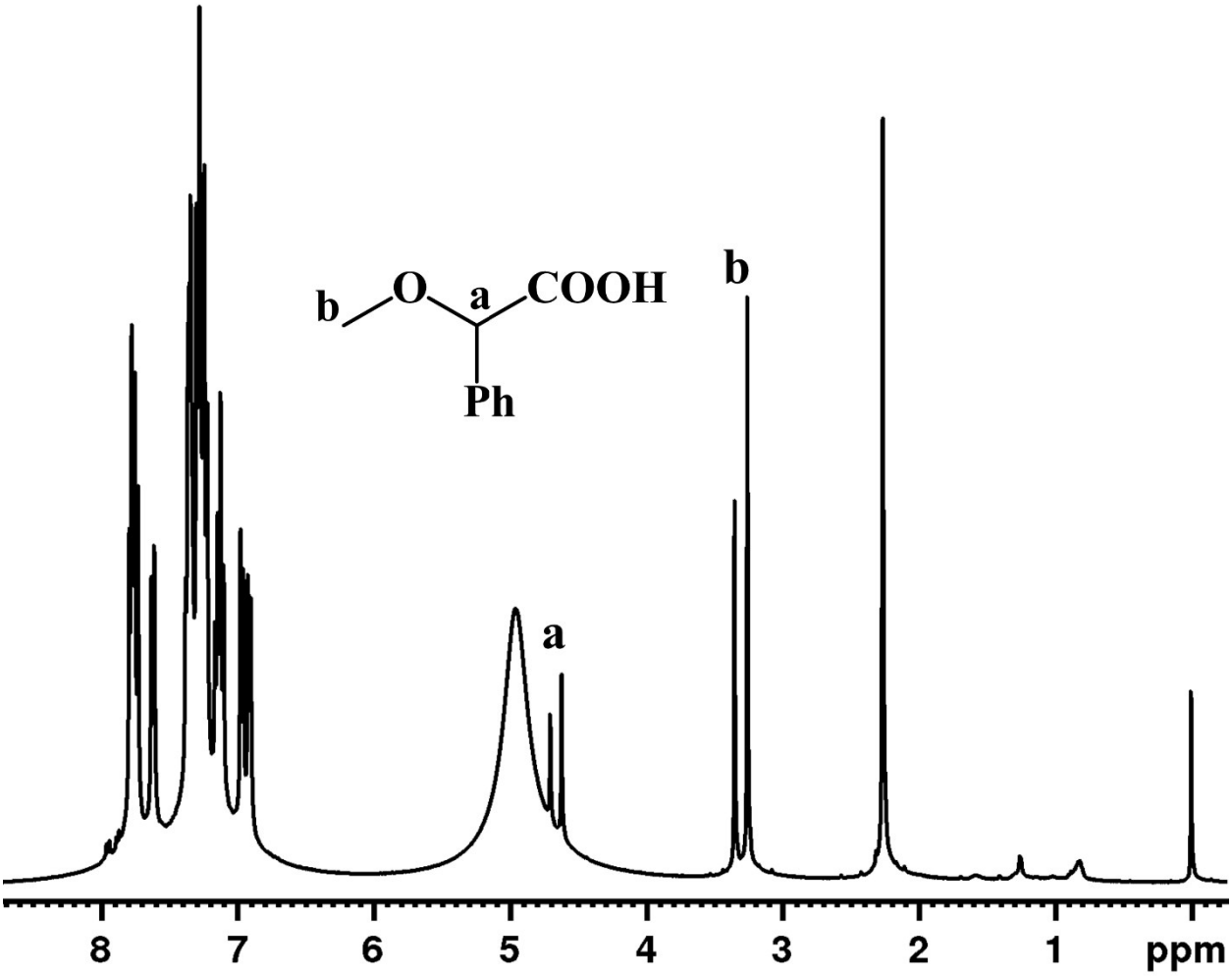


S18

376 MHz ^{19}F-NMR spectrum of (*R/S*)-α-Methoxy-α-(trifluoromethyl) phenylacetic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$

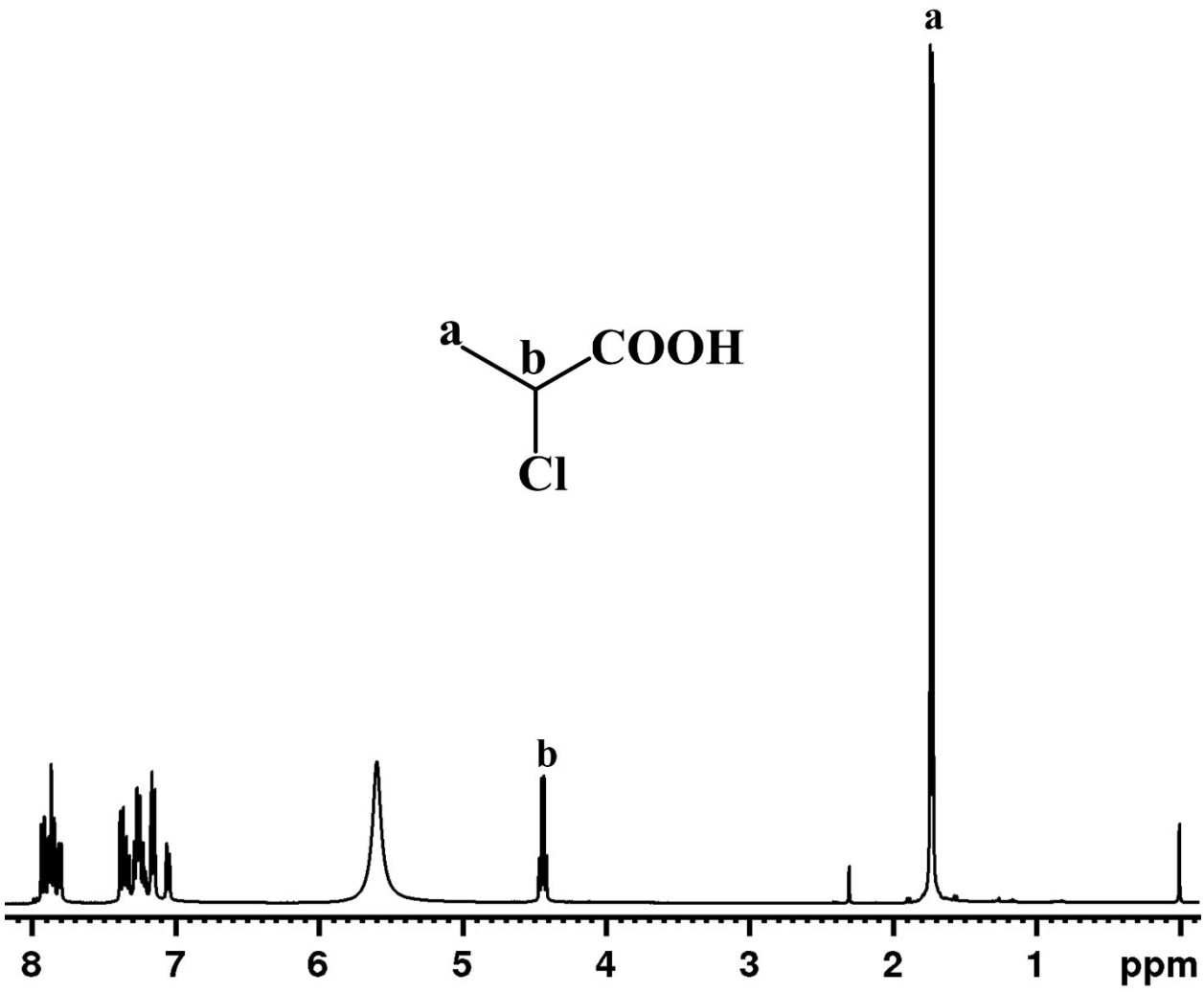


400 MHz ^{1}H-NMR spectrum of (*R/S*)-2-Methoxy-2-phenylacetic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$

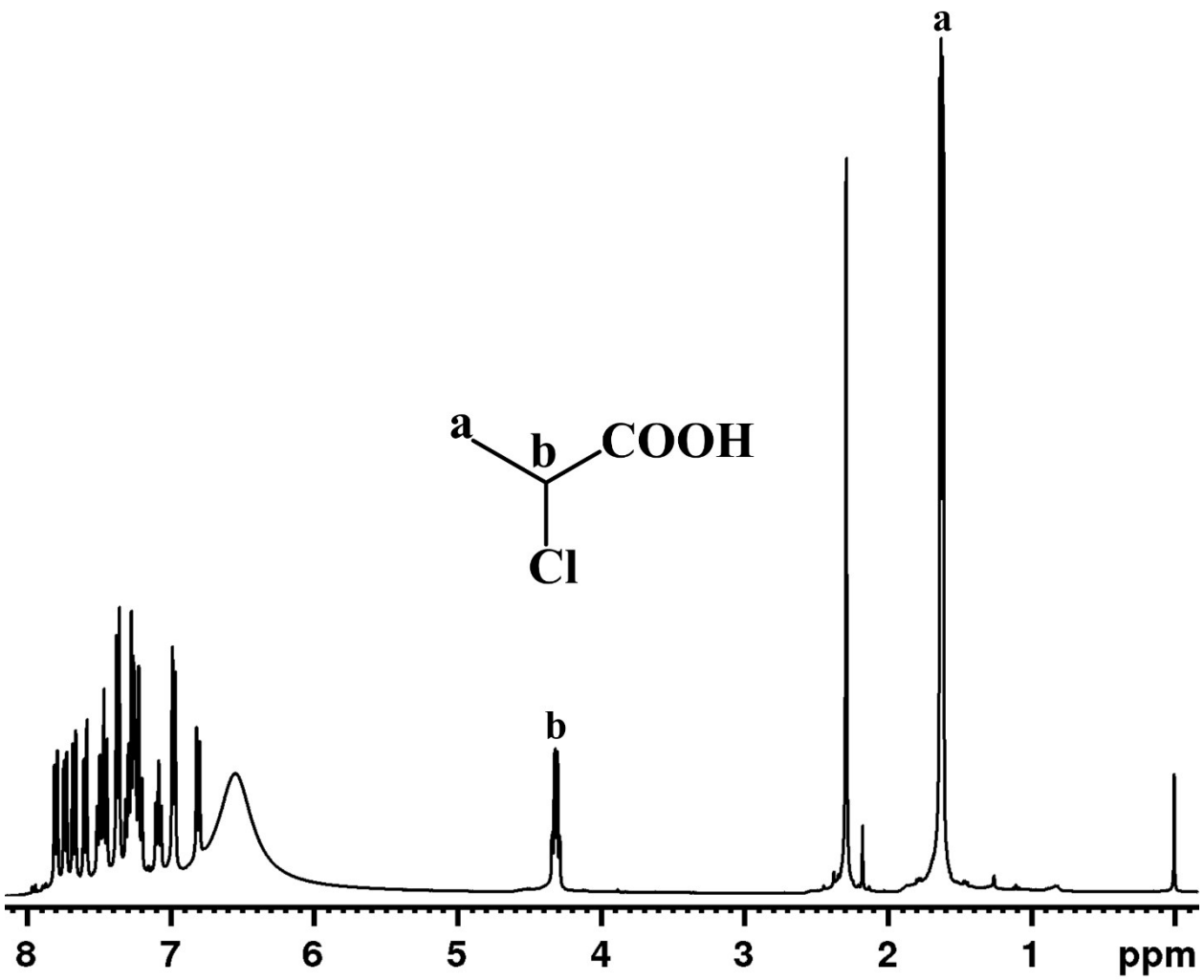


S20

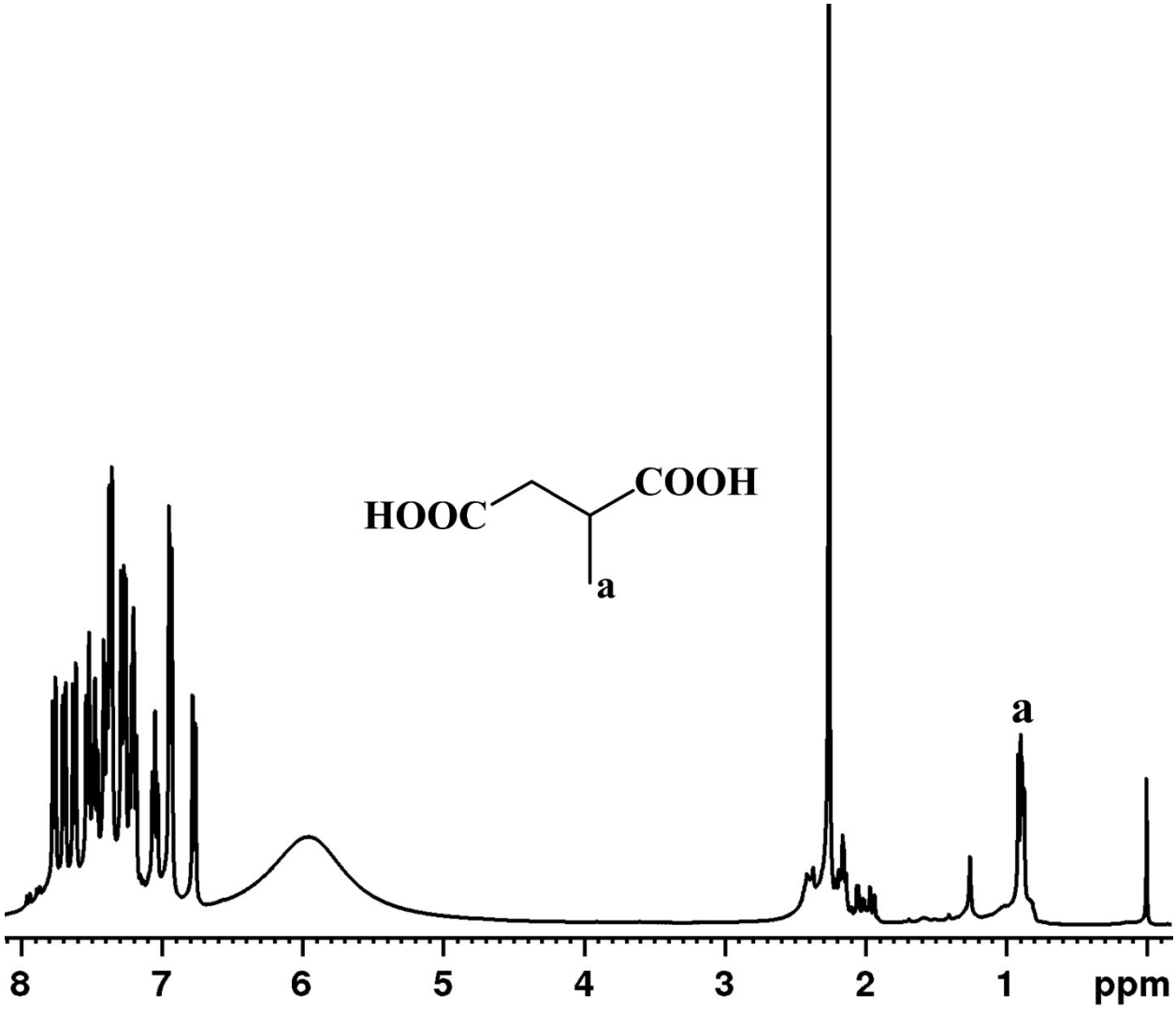
400 MHz ^{1}H-NMR spectrum of (*R/S*)-2-Chloro propanoic acid and (*R*)-NOBIN in $CDCl_3$



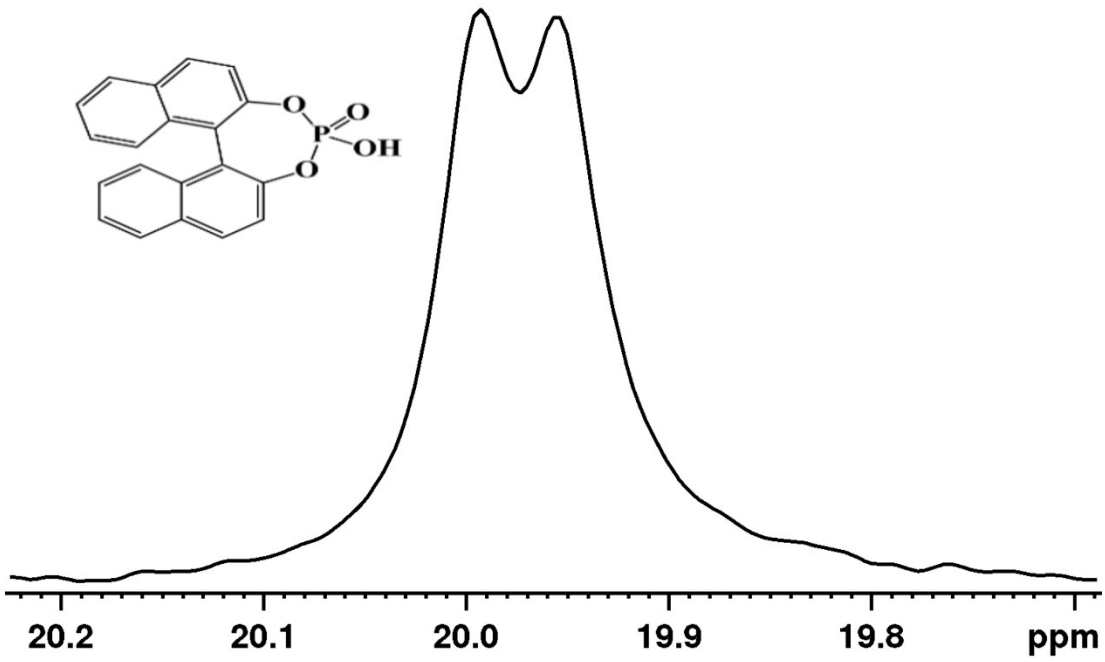
400 MHz ^{1}H-NMR spectrum of (*R/S*)-2-Chloro propionic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



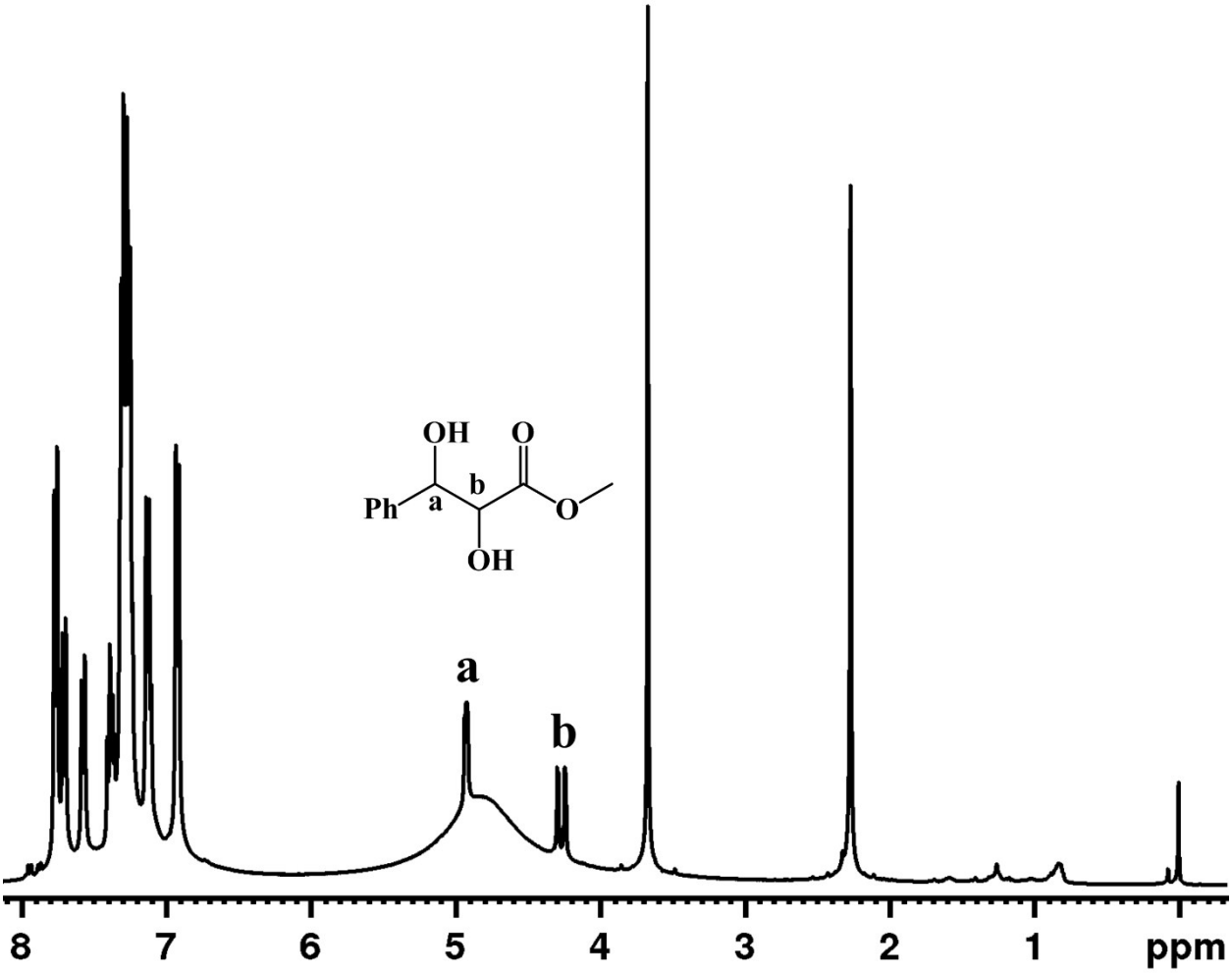
400 MHz ^{1}H-NMR spectrum of (*R/S*) -Methylsuccinic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



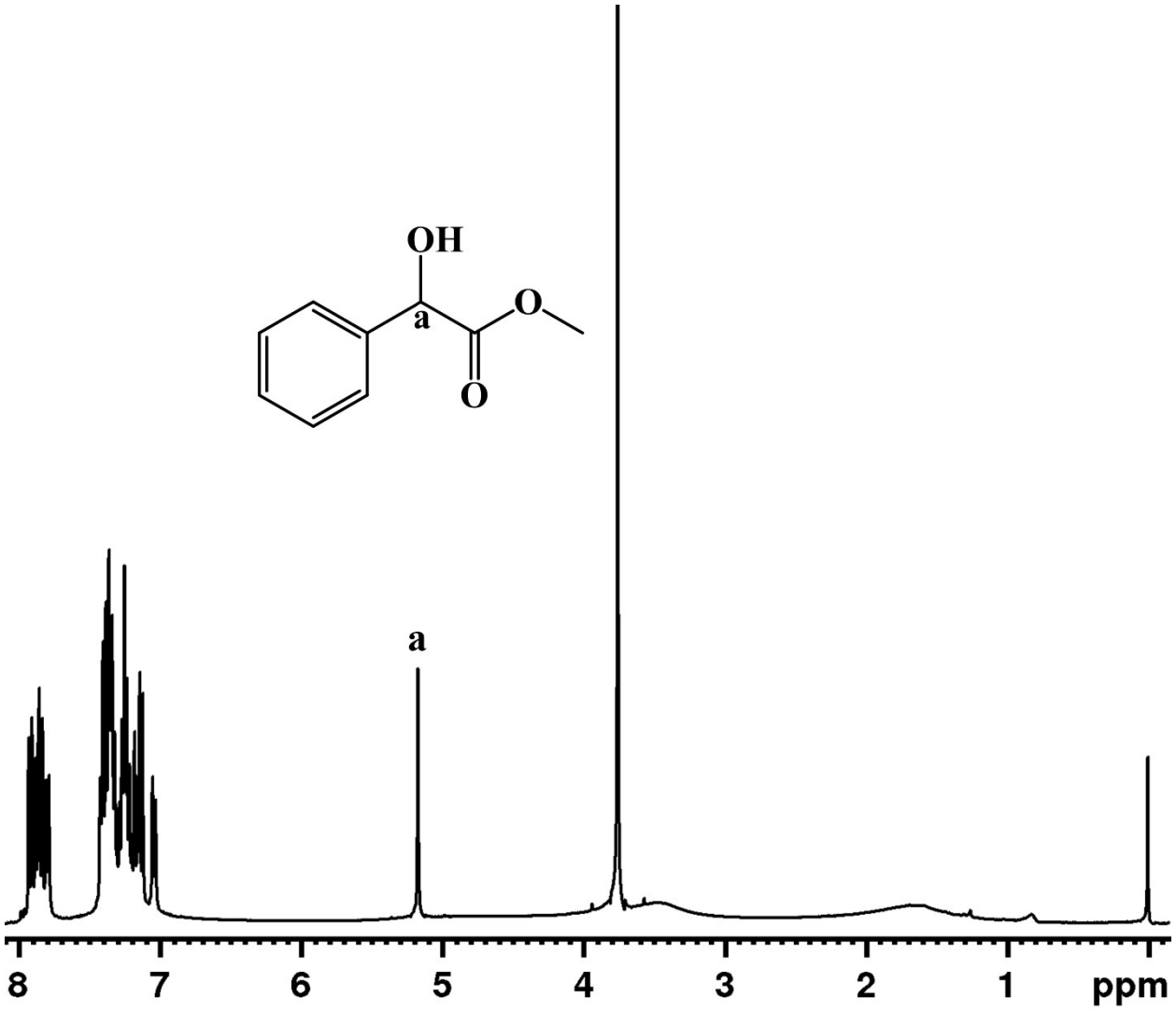
161.9 MHz ^{31}P-NMR spectrum of (*R/S*) -1, 1′-Binaphthyl-2, 2′-diyl hydrogenphosphate, (*R*)-NOBIN and p-TsOH in $CDCl_3$



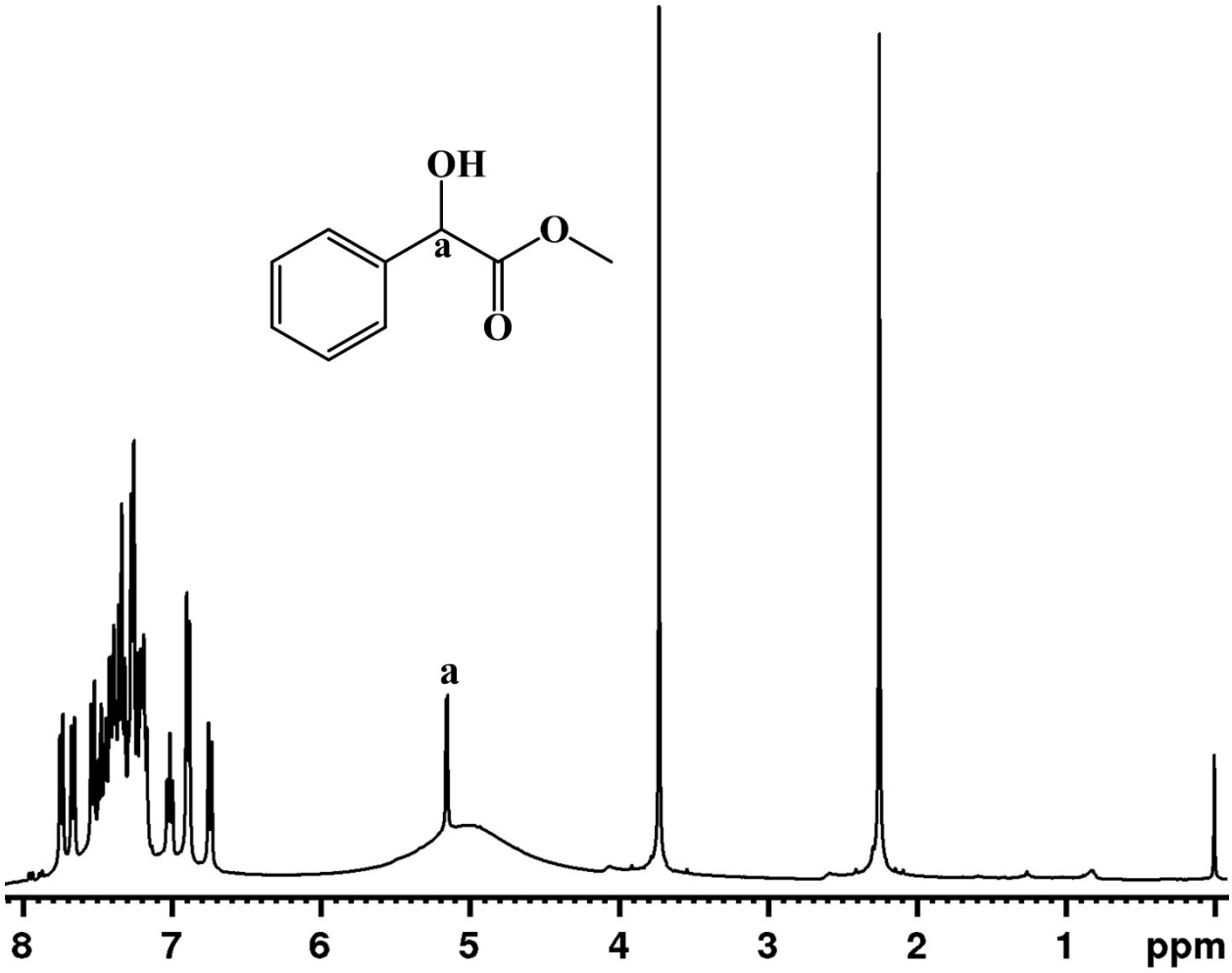
400 MHz ^{1}H-NMR spectrum of (*R/S*)-Methyl 2, 3 dihydroxy 3-phenyl propionate, (*R*)-NOBIN and p-TsOH in $CDCl_3$



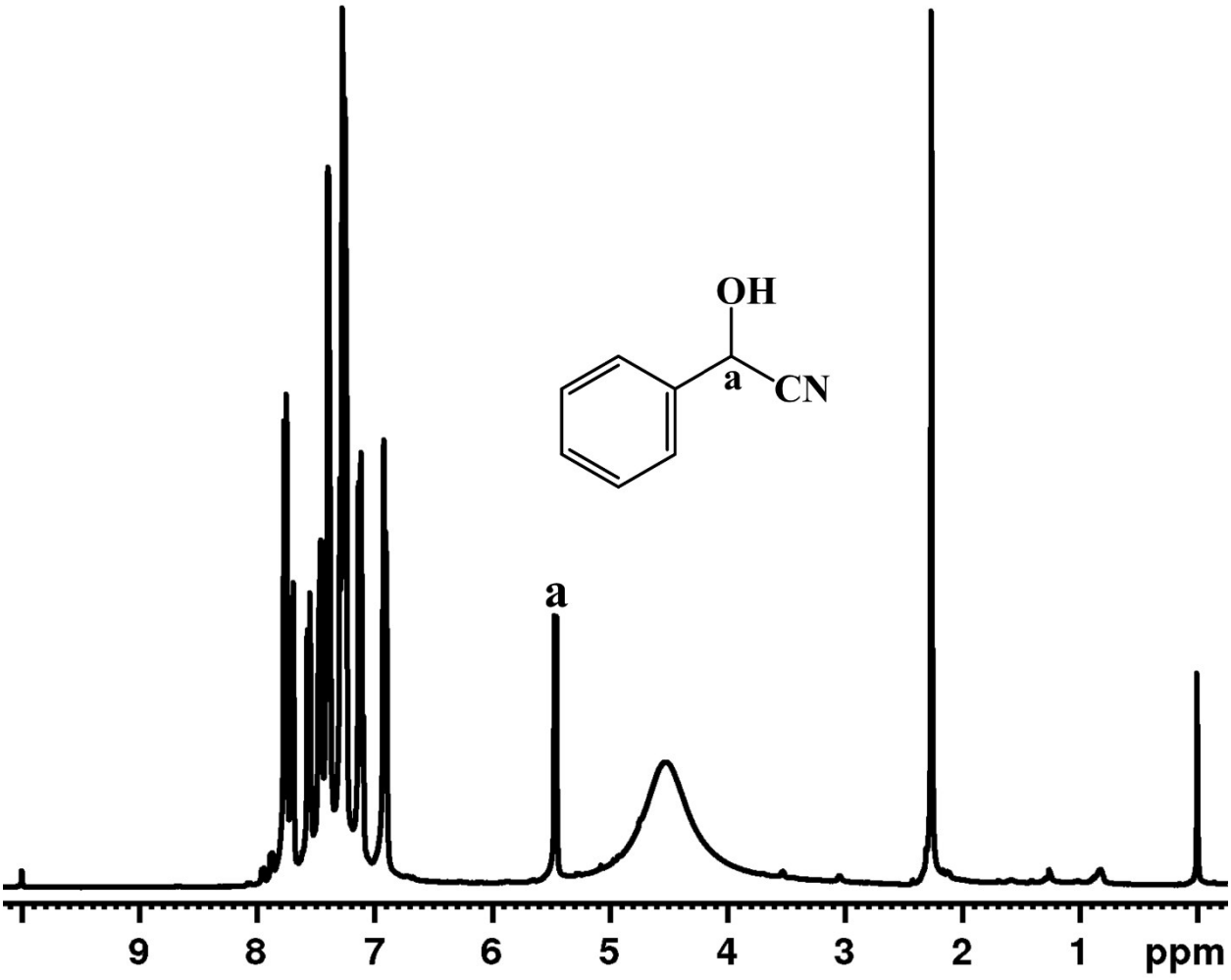
400 MHz ^{1}H-NMR spectrum of (*R/S*)-Methyl mandelate and (*R*)-NOBIN in $CDCl_3$



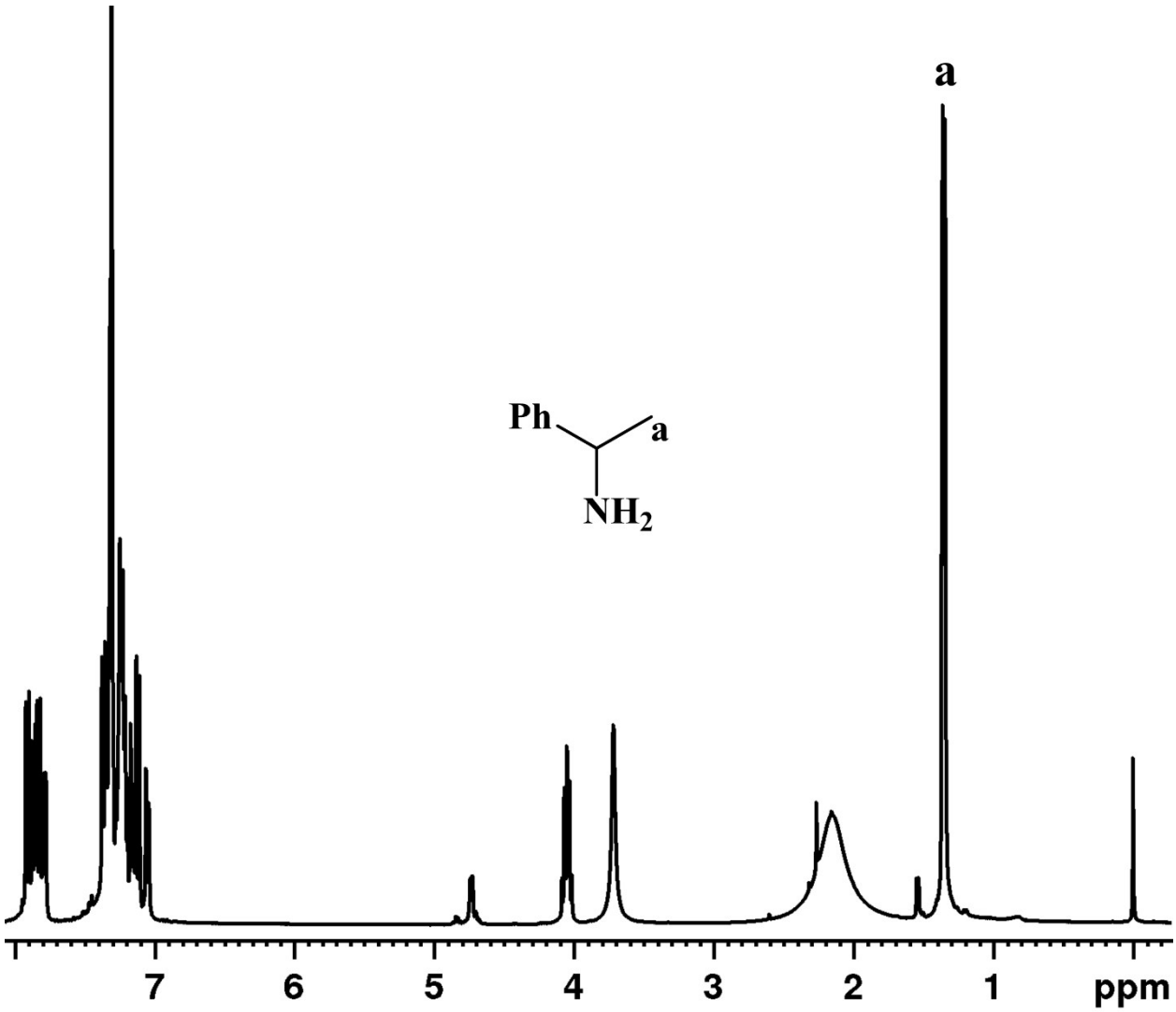
400 MHz ^{1}H-NMR spectrum of (*R/S*) -Methyl mandelate, (*R*)-NOBIN and p-TsOH in $CDCl_3$



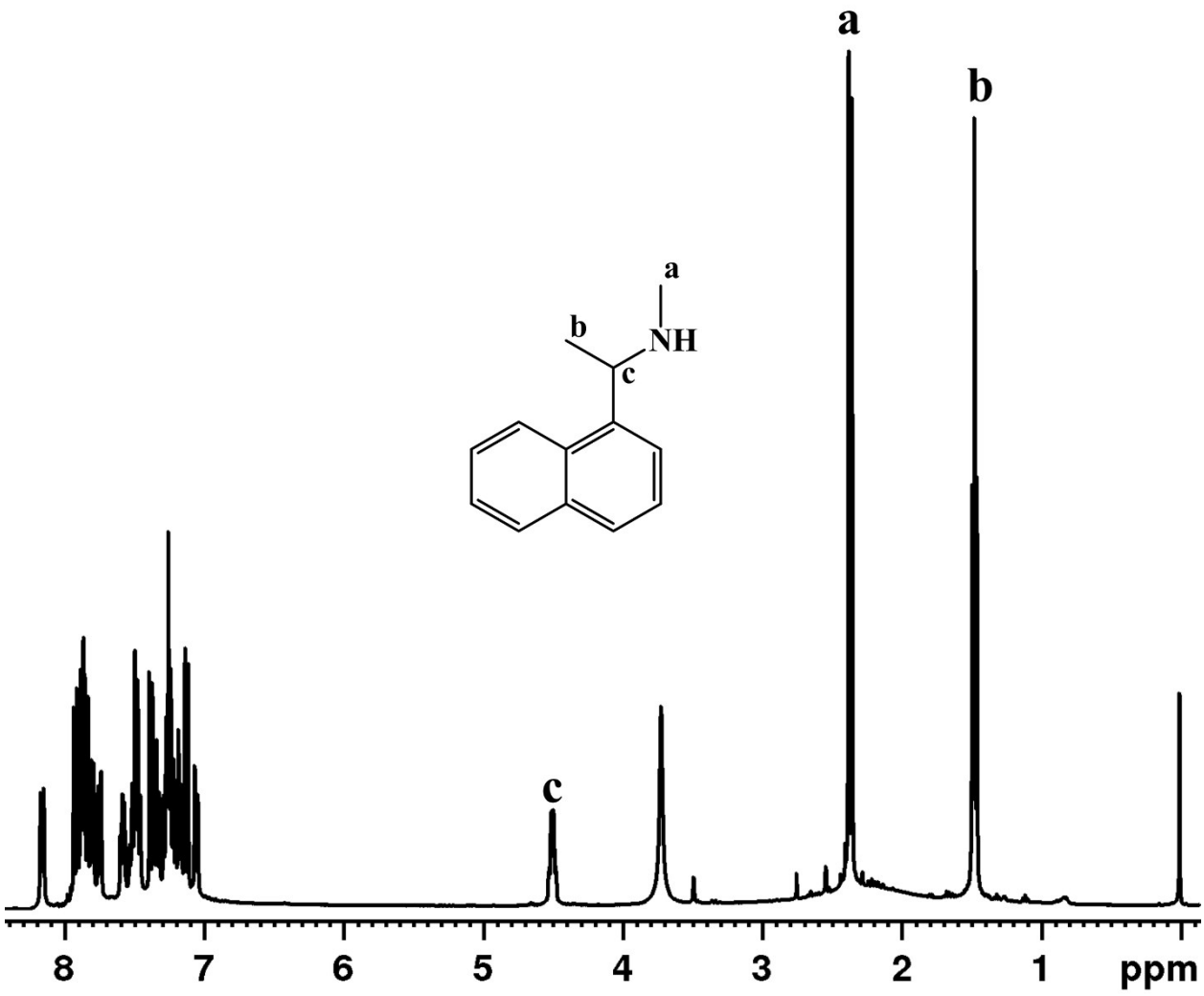
400 MHz ^{1}H-NMR spectrum of (*R/S*) -Mandelonitrile, (*R*)-NOBIN and p-TsOH in $CDCl_3$



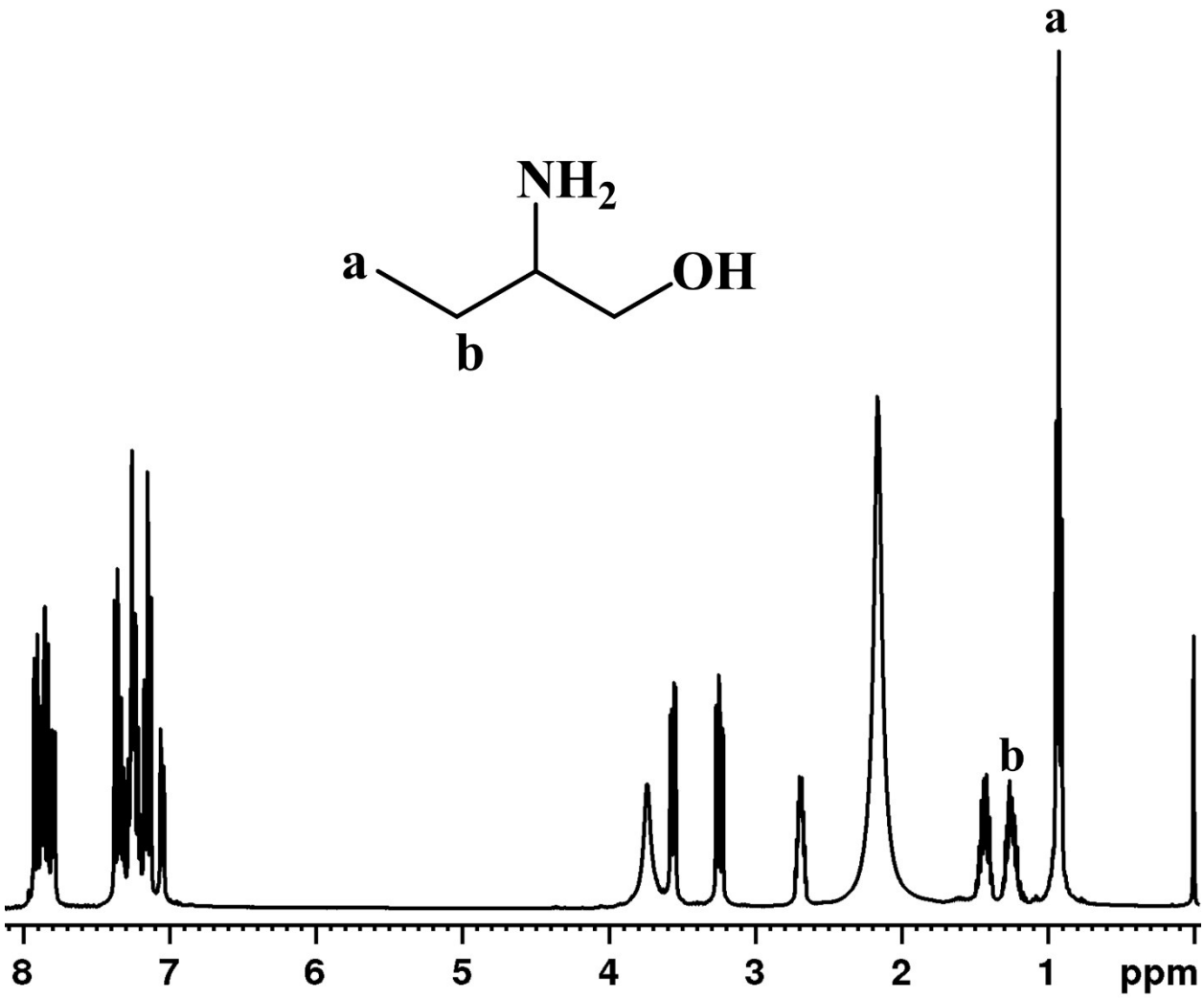
400 MHz ^{1}H-NMR spectrum of (*R/S*) -alpha Methyl benzyl amine, (*R*)-NOBIN in $CDCl_3$



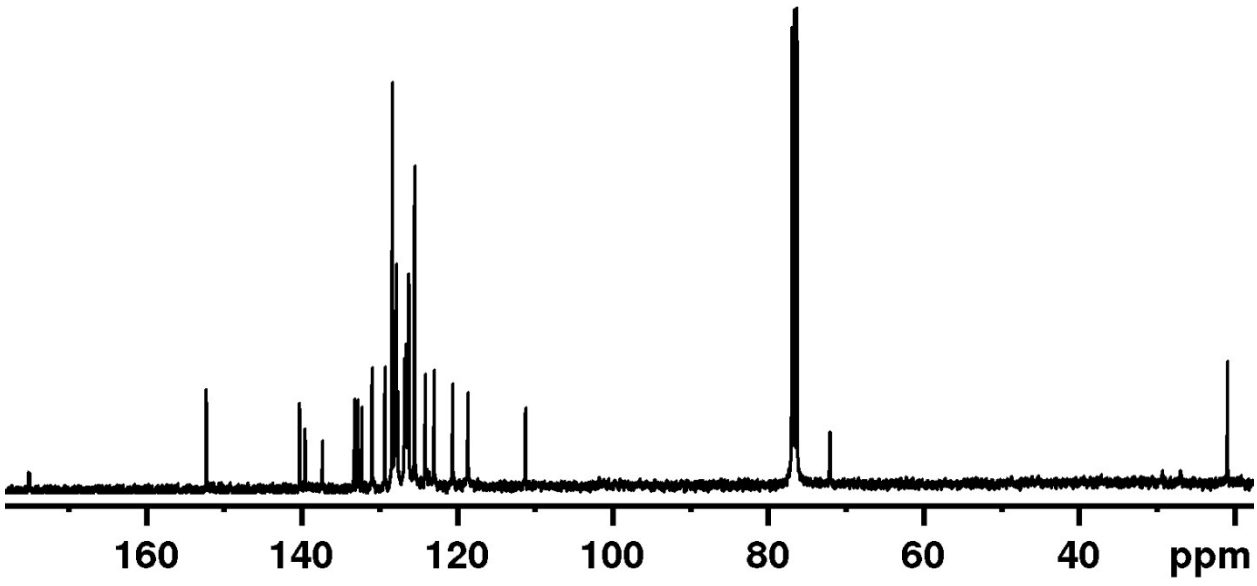
400 MHz ^{1}H-NMR spectrum of (*R/S*)-N-Methyl-1-(1-naphthyl) ethylamine, (*R*)-NOBIN in $CDCl_3$



400 MHz ^{1}H-NMR spectrum of (*R/S*)-2-amino 1-butanol, (*R*)-NOBIN in $CDCl_3$

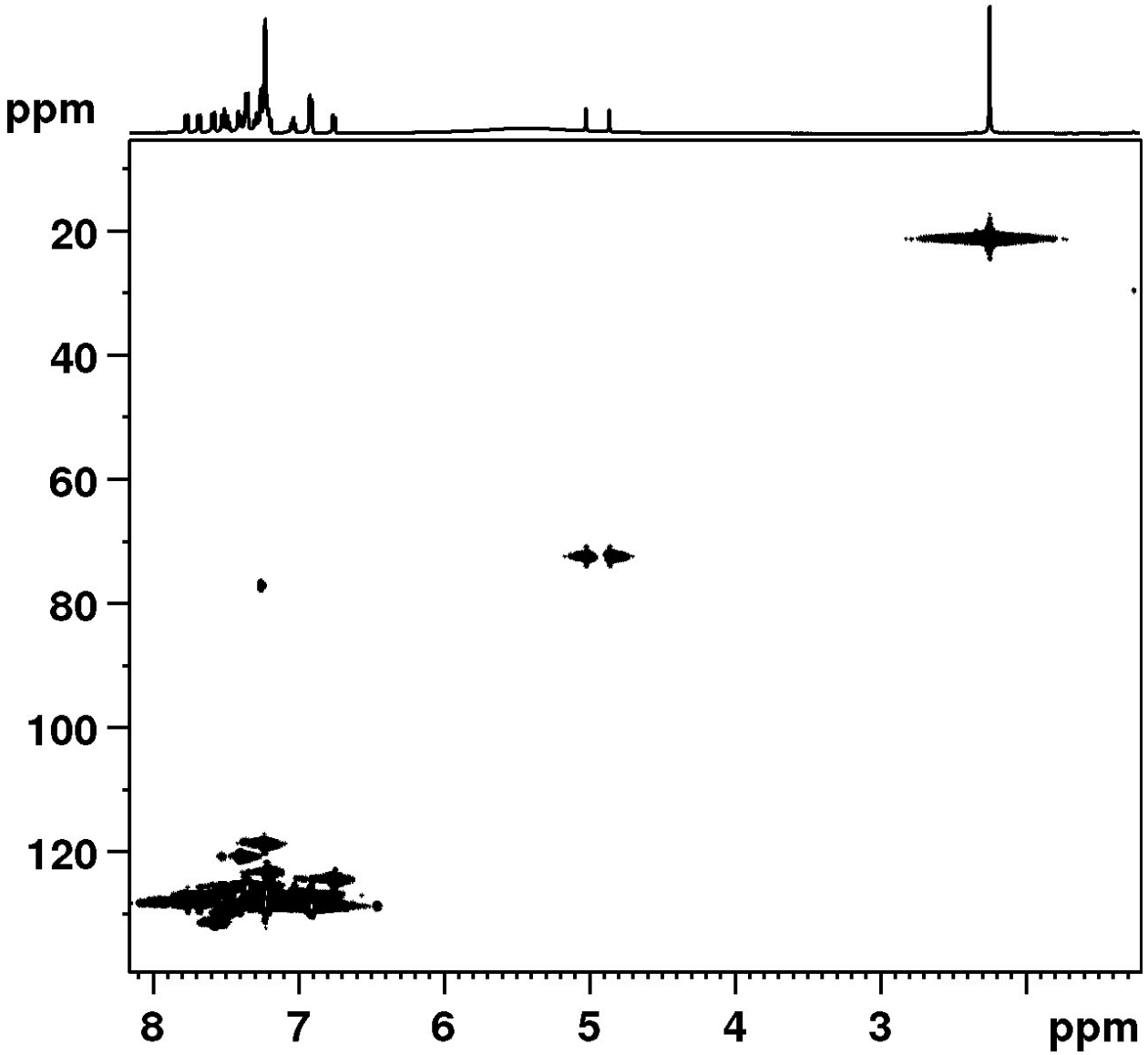


100 MHz ^{13}C spectrum of (*R/S*) - Mandelic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$

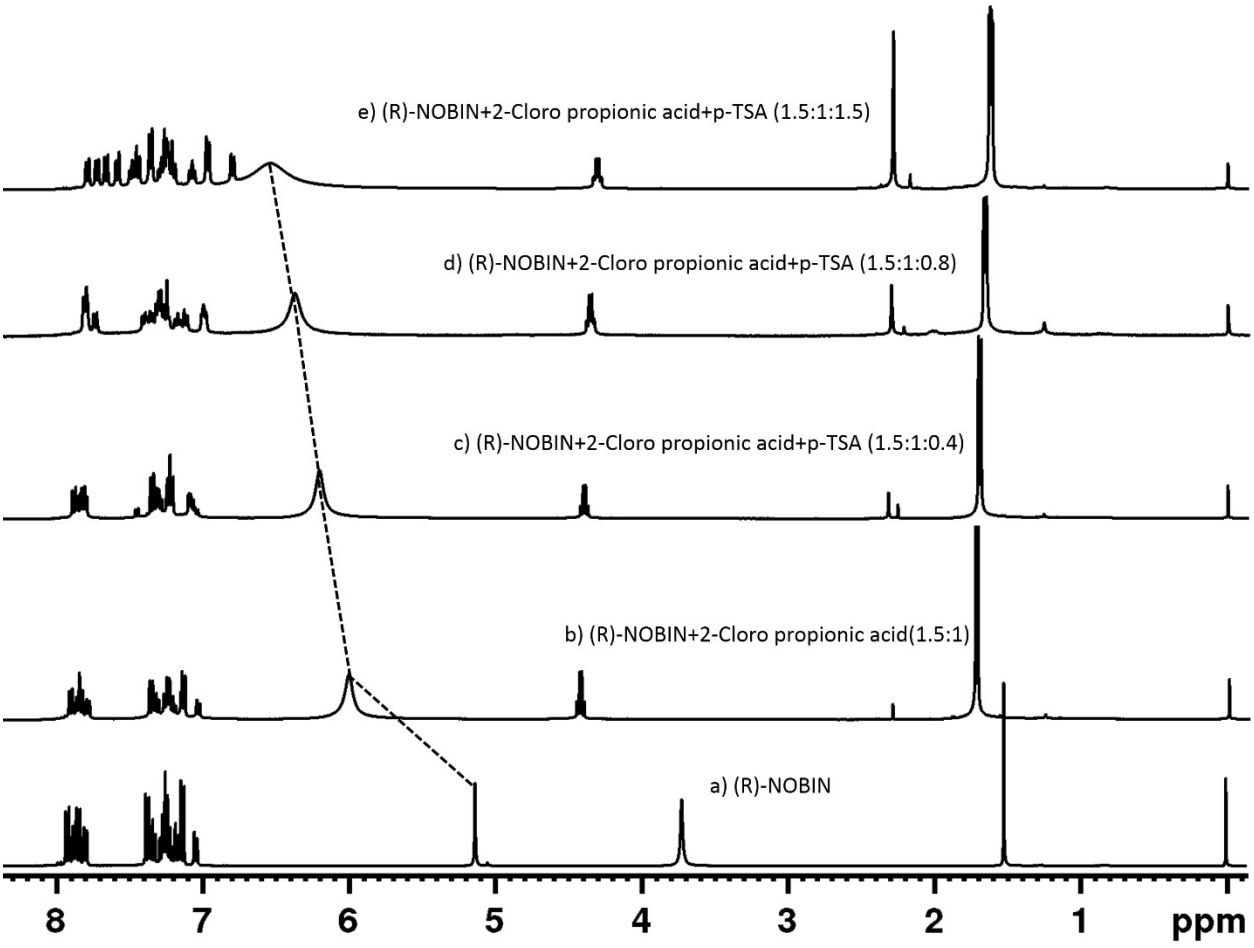


S32

500 MHz HSQC spectrum of (*R/S*) - Mandelic acid, (*R*)-NOBIN and p-TsOH in $CDCl_3$



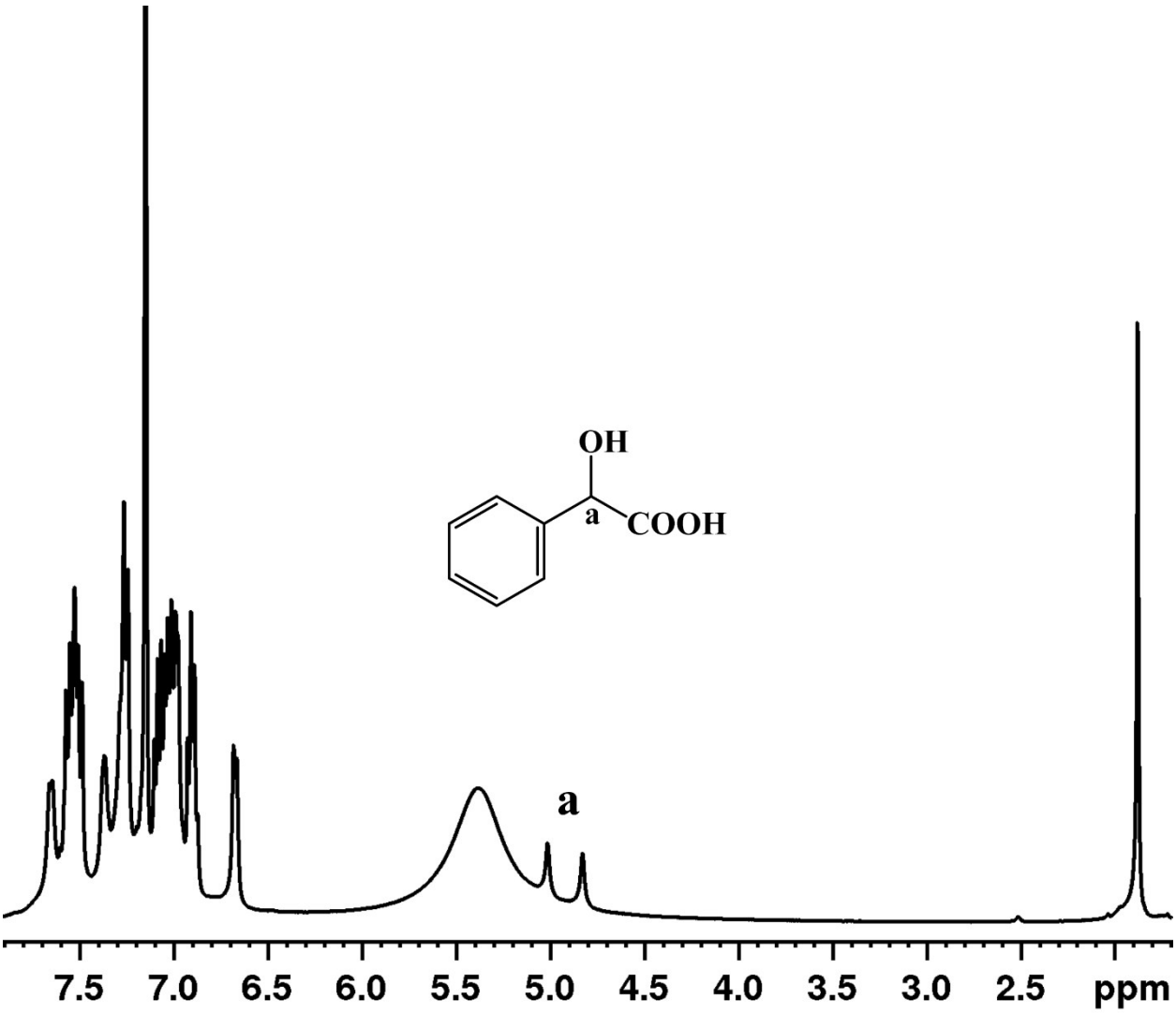
Stack plot of ^{1}H-NMR spectrum of (*R*)-NOBIN (a), 2-Chloro propionic acid and (*R*)-NOBIN (b), 2-Chloro propionic acid, (*R*)-NOBIN and different equivalents of p-TsOH (c, d, e) in $CDCl_3$ showing the deshielding of OH-group of (*R*)-NOBIN with dashed lines.



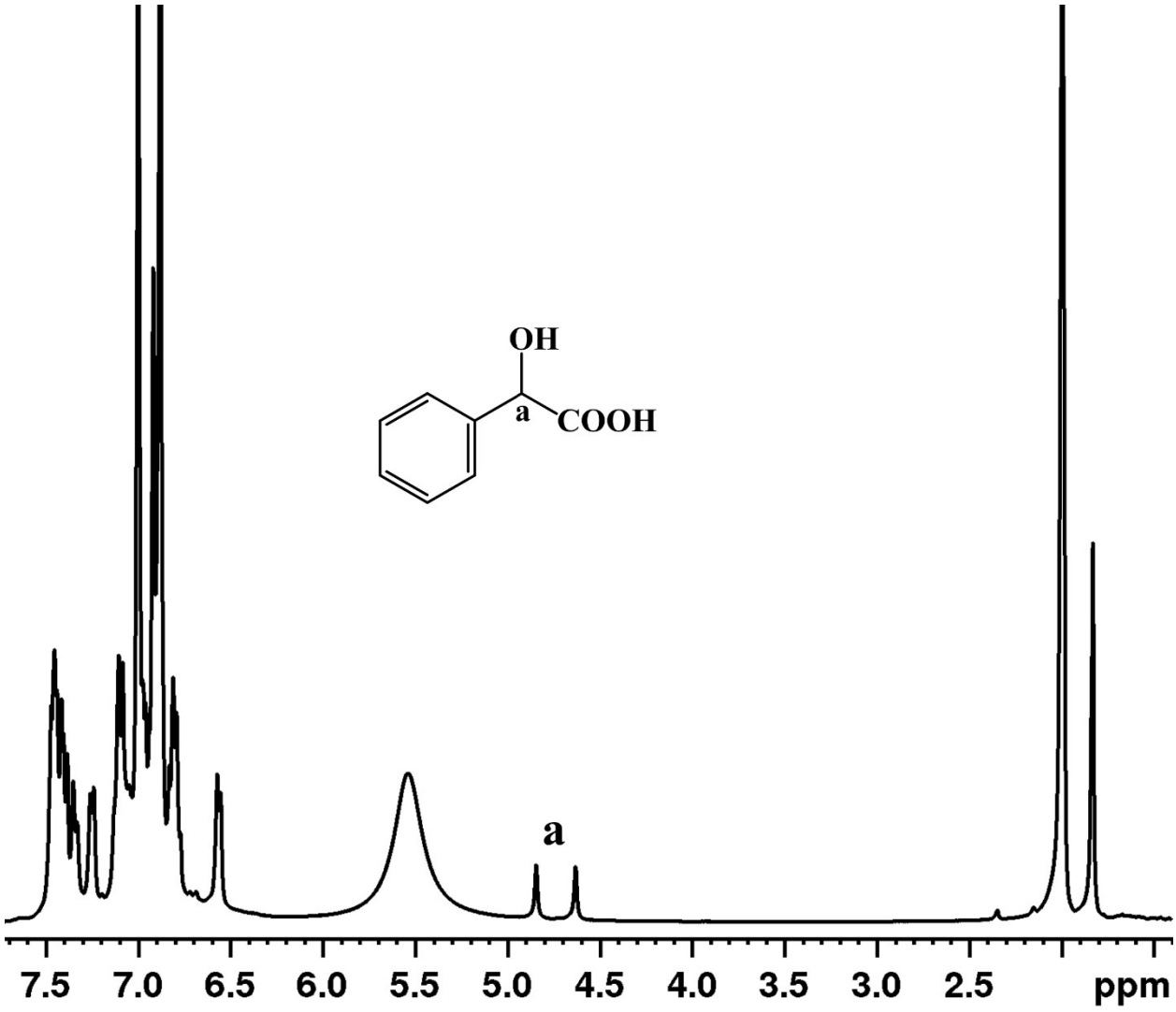
Chemical shift difference for the selected proton of (*R/S*)-Mandelic acid in presence of (*R*)-NOBIN and p-TsOH in different solvents

S.No	Solvent	*Δδ R/S* (ppm)
1	CDCl3	0.21
2	C6D6	0.19
3	TOLUENE-d8	0.21
4	CD2Cl2	0.13

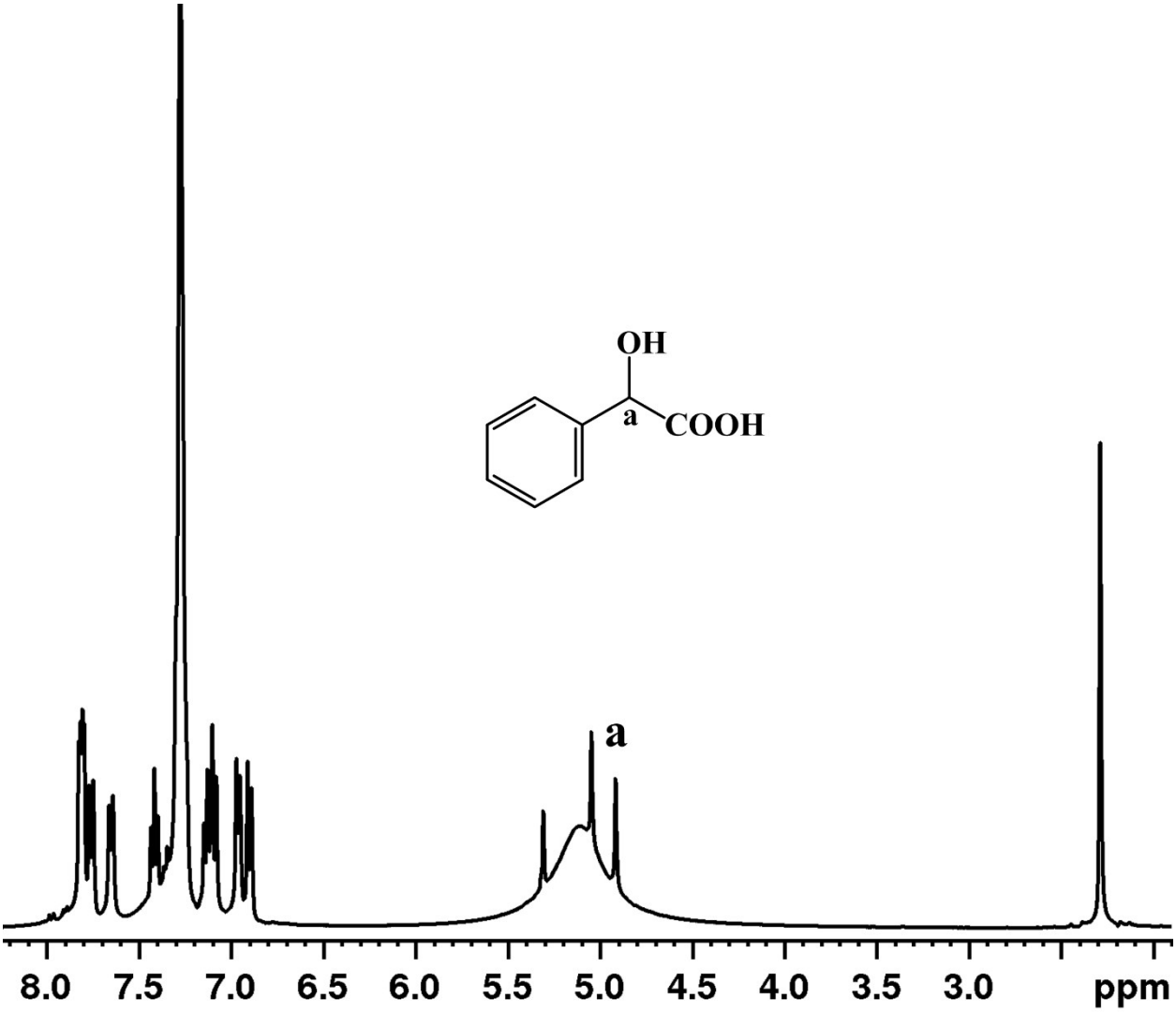
400 MHz ^{1}H-NMR spectrum of (*R/S*) -Mandelic acid, (*R*)-NOBIN and p-TsOH in C_6D_6



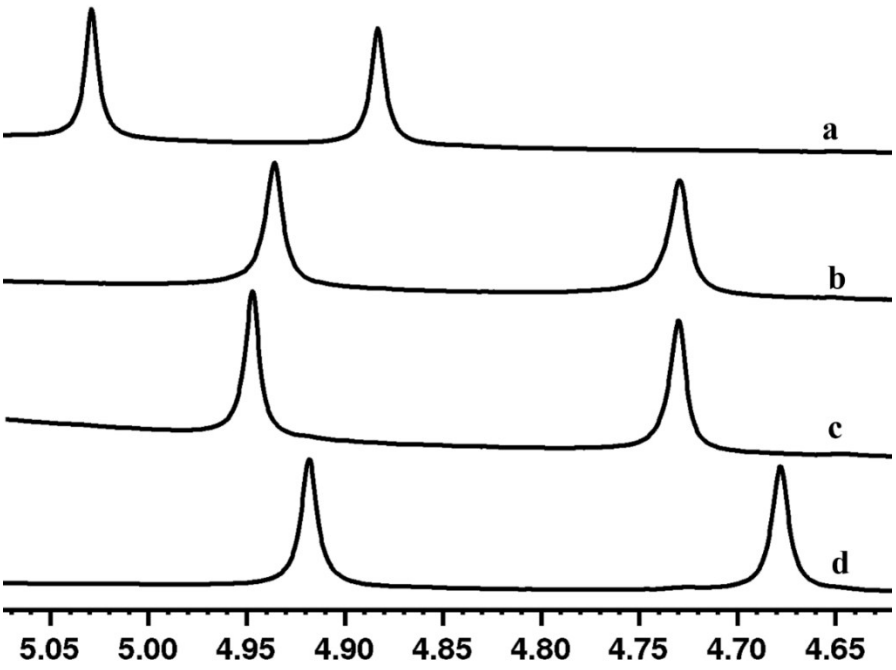
400 MHz ^{1}H-NMR spectrum of (*R/S*) -Mandelic acid, (*R*)-NOBIN and p-TsOH in in toluene-d_8 (C_7D_8)



400 MHz ^{1}H-NMR spectrum of (*R/S)* -Mandelic acid, (*R*)-NOBIN and p-TsOH in methylenechloride-d_2 (CD_2Cl_2)



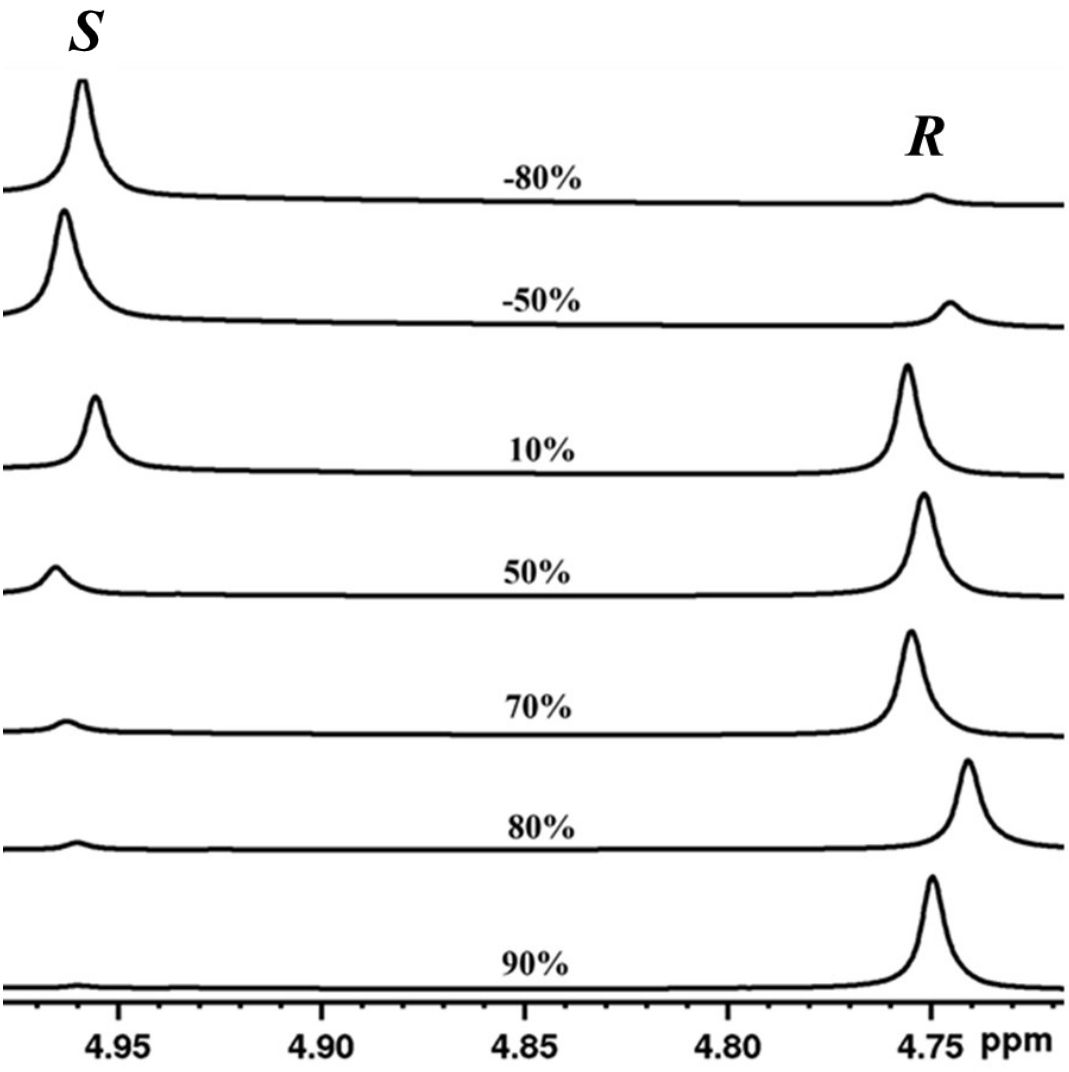
400 MHz ^{1}H-NMR spectrum pertaining to alpha proton of (*R/S*) – Mandelic acid; (a-d) with 1:1:1, 1:2:2, 1:3:3 and 1:4:4 equivalents of (*R/S*) – Mandelic acid and (*R*)-NOBIN, p-TsOH in $CDCl_3$



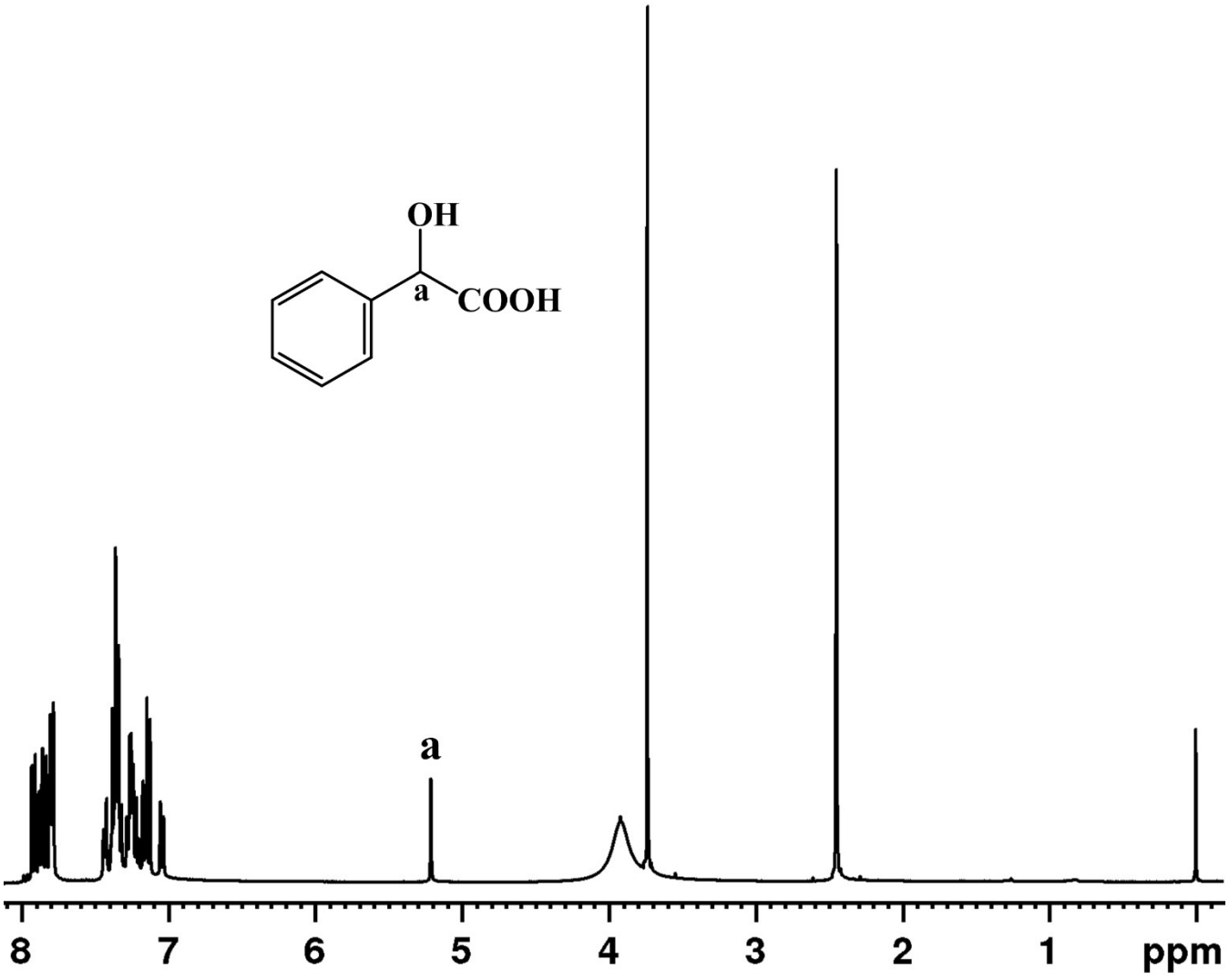
The experimentally determined and laboratory prepared scalemic ratios of (*R/S*) – Mandelic acid and (*R*)-NOBIN in presence of p-TsOH. Alpha proton was chossen for *ee* measurements.

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	1.000:0.8172	10	10.06
2	1.000:0.3275	50	50.6
3	1.000:0.1758	70	70.097
4	1.000:0.1017	80	80.6
5	1.000:0.0512	90	89.17
6	1.000:3.0280	-50	-50.3
7	1.000:8.683	-80	-79.4

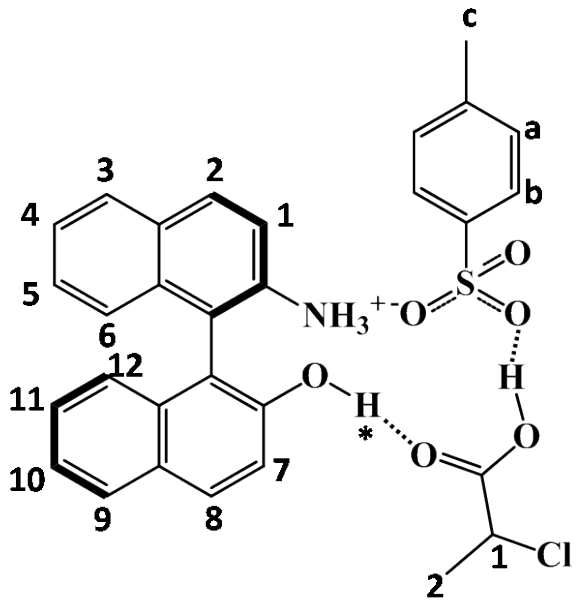
400 MHz ^{1}H-NMR spectra of selected regions of different scalemic ratios of *R*–Mandelic acid and (*S)*-Mandelic acid in presence of (*R*)-NOBIN in presence of p-TsOH in $CDCl_3$



400 MHz ^{1}H-NMR spectrum of (*R/S*)-Mandelic acid, (*R*)-NOBIN and Methyl p-Toluenesulfonate in $CDCl_3$

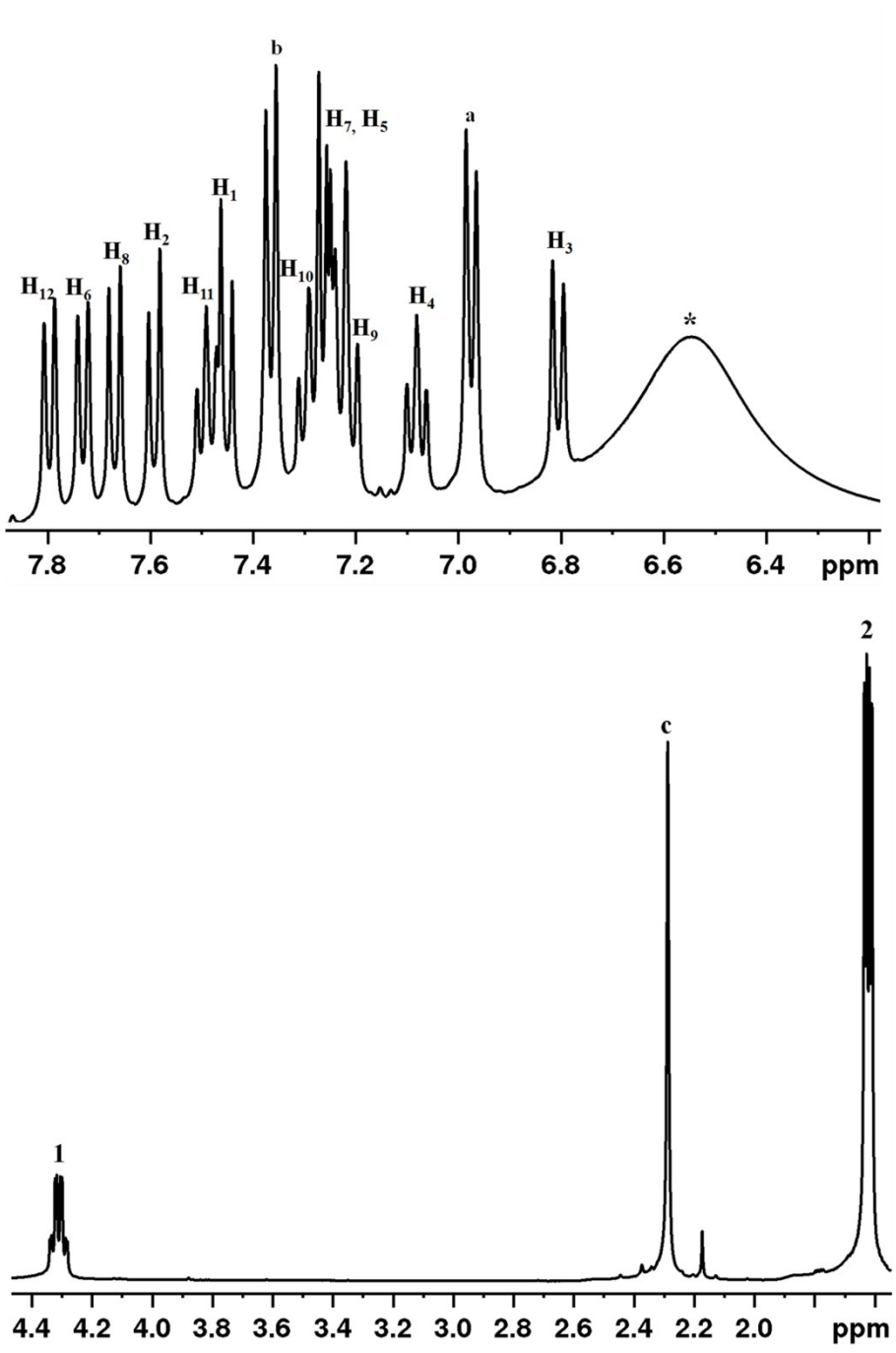


(*R/S*) - 2-Chloro propanoic acid, (*R*)-NOBIN and p-TsOH ternary ion structure with lables



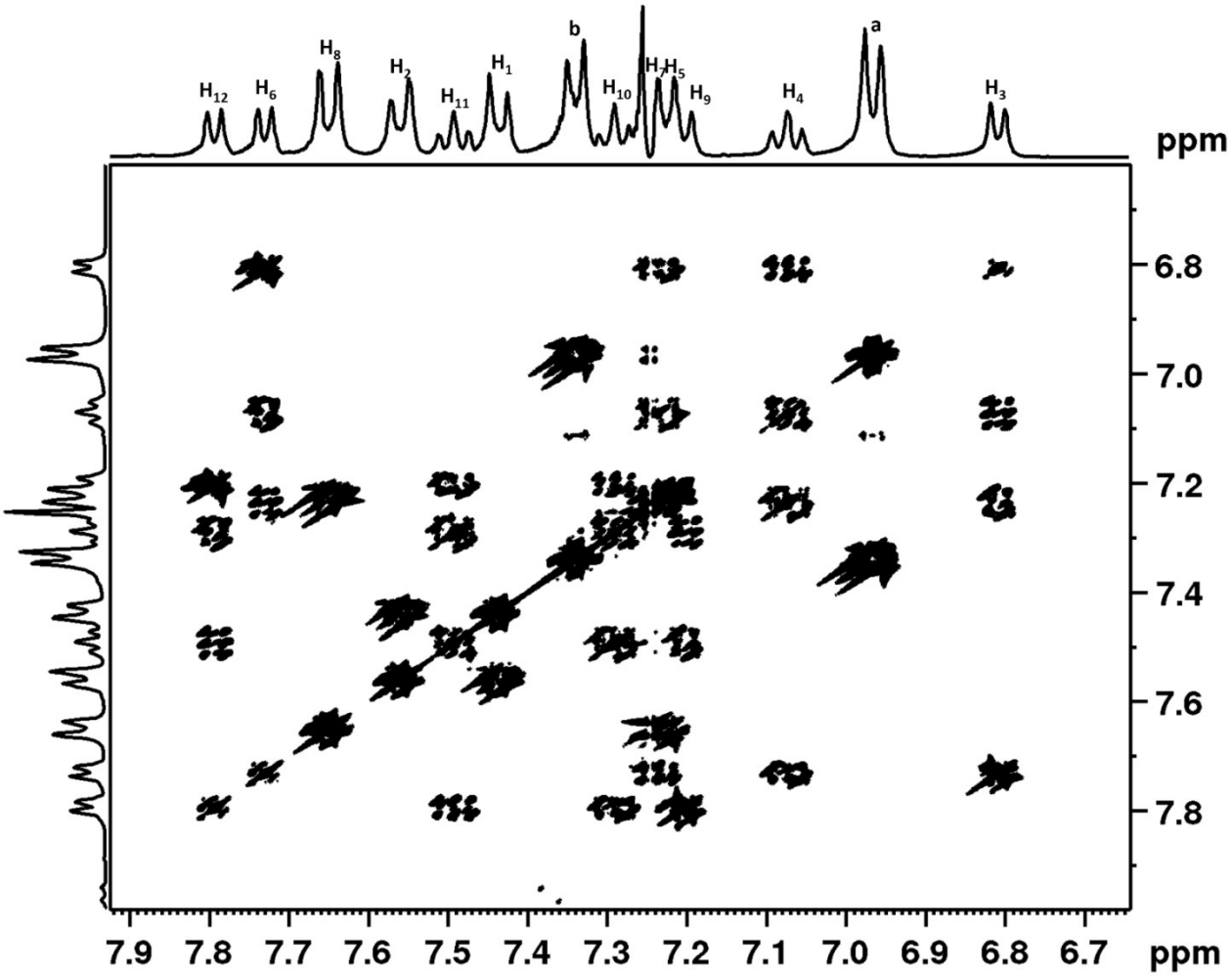
S43

400 MHz ^{1}H-NMR spectrum of (*R/S*) - 2-Chloro propanoic acid, (*R*)-NOBIN and p-TsOH (1:1:1) in $CDCl_3$ with assignments made by TOCSY, COSY and ^{1}H and ^{13}C HSQC

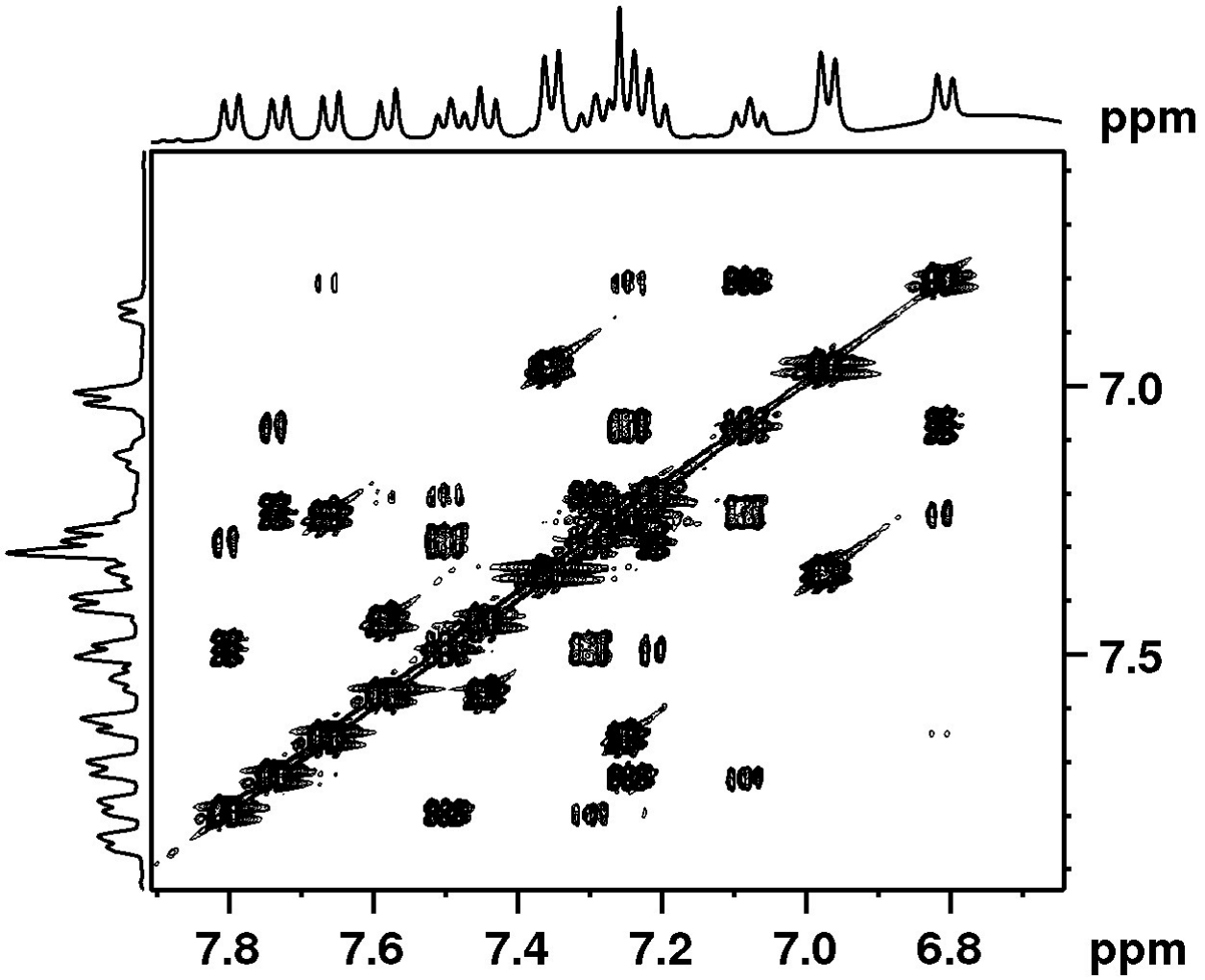


S44

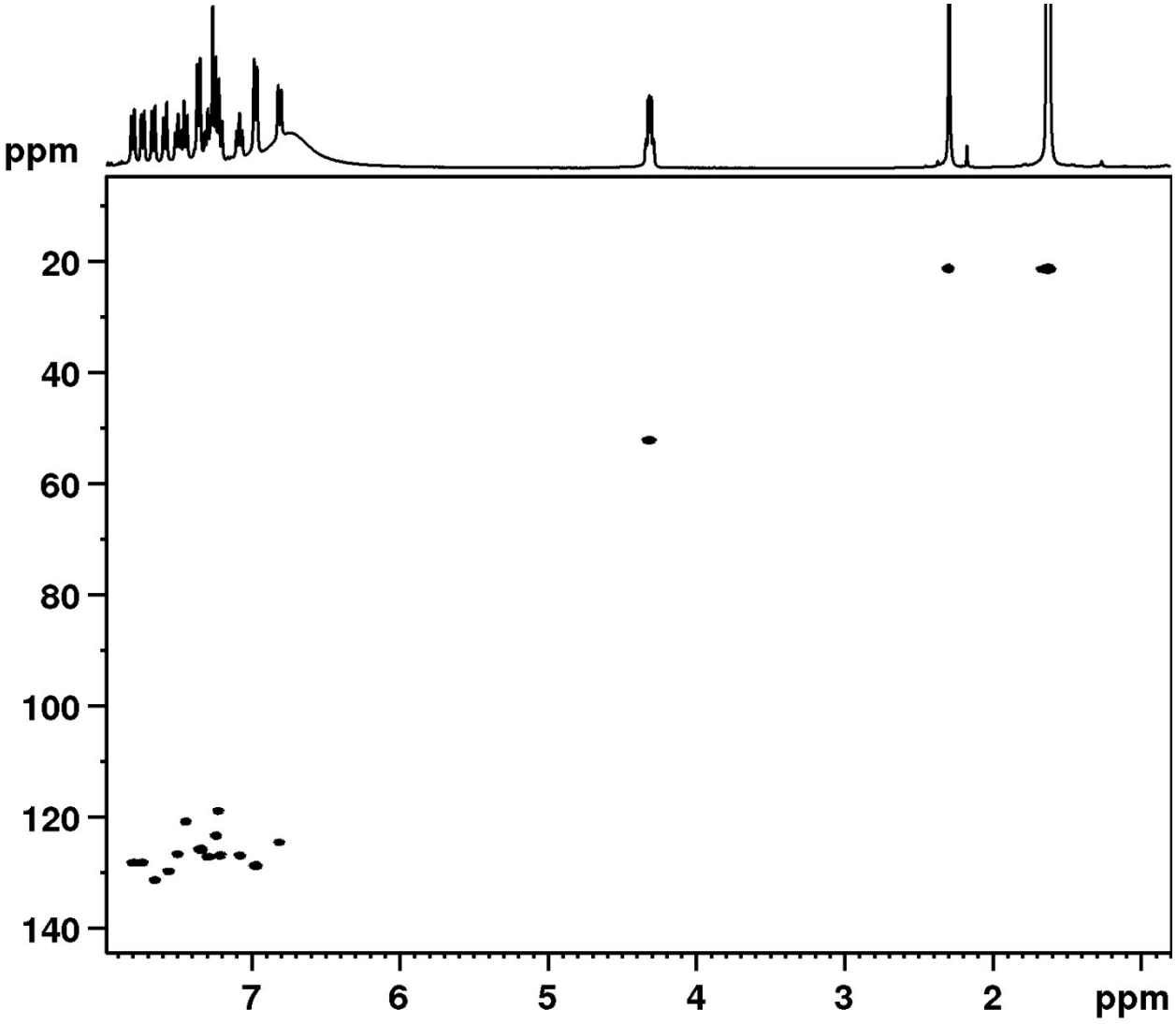
400 MHz TOCSY spectrum of (*R/S*) - 2-Chloro propanoic acid, (*R*)-NOBIN and p-TsOH (1:1:1) in $CDCl_3$



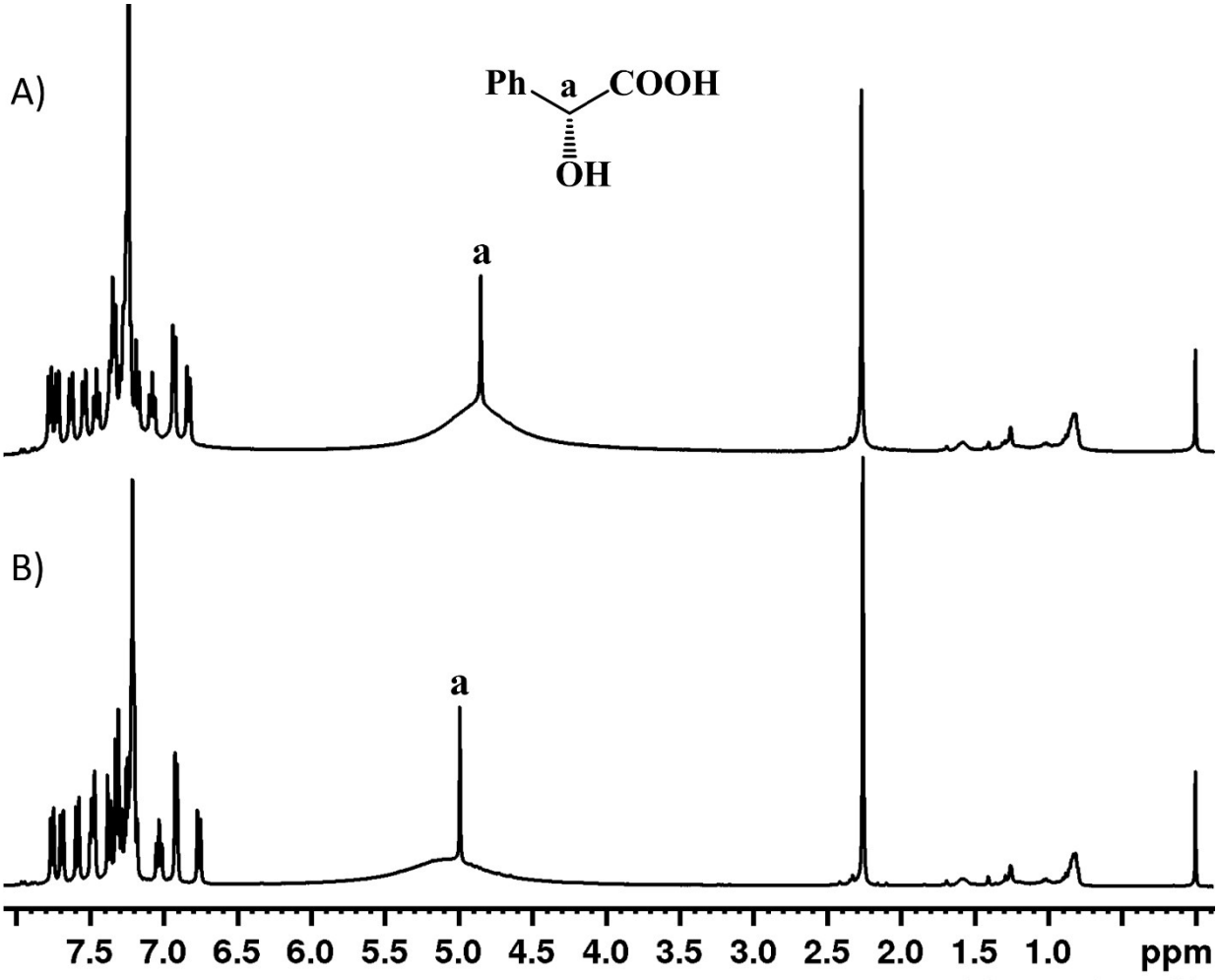
400 MHz COSY spectrum of (*R/S*)-2-Chloro propanoic acid, (*R*)-NOBIN and p-TsOH (1:1:1) in $CDCl_3$



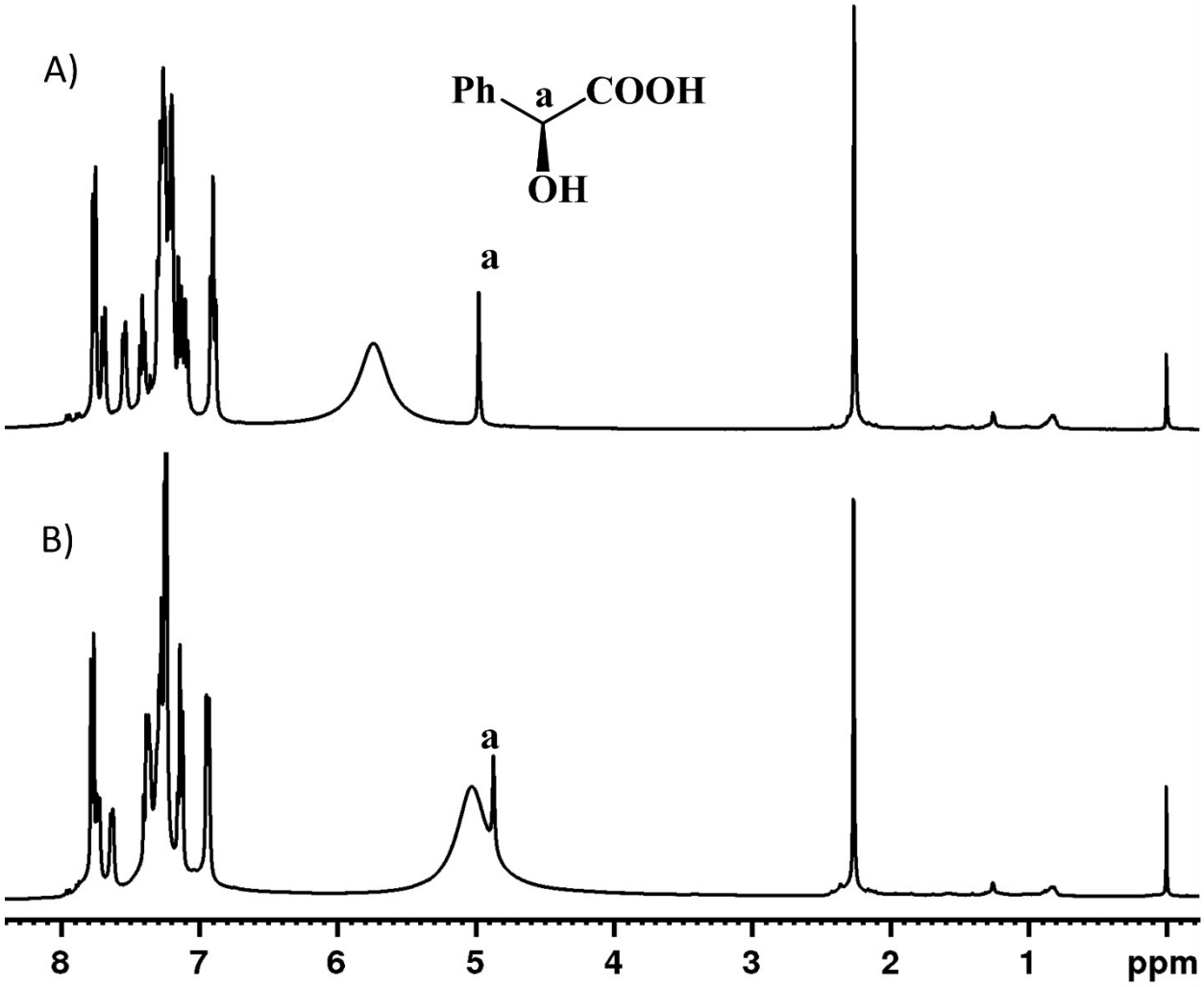
400 MHz ^{1}H and ^{13}C HSQC spectrum of (*R/S*)-2-Chloro propanoic acid, (*R*)-NOBIN and p-TsOH (1:1:1) in $CDCl_3$



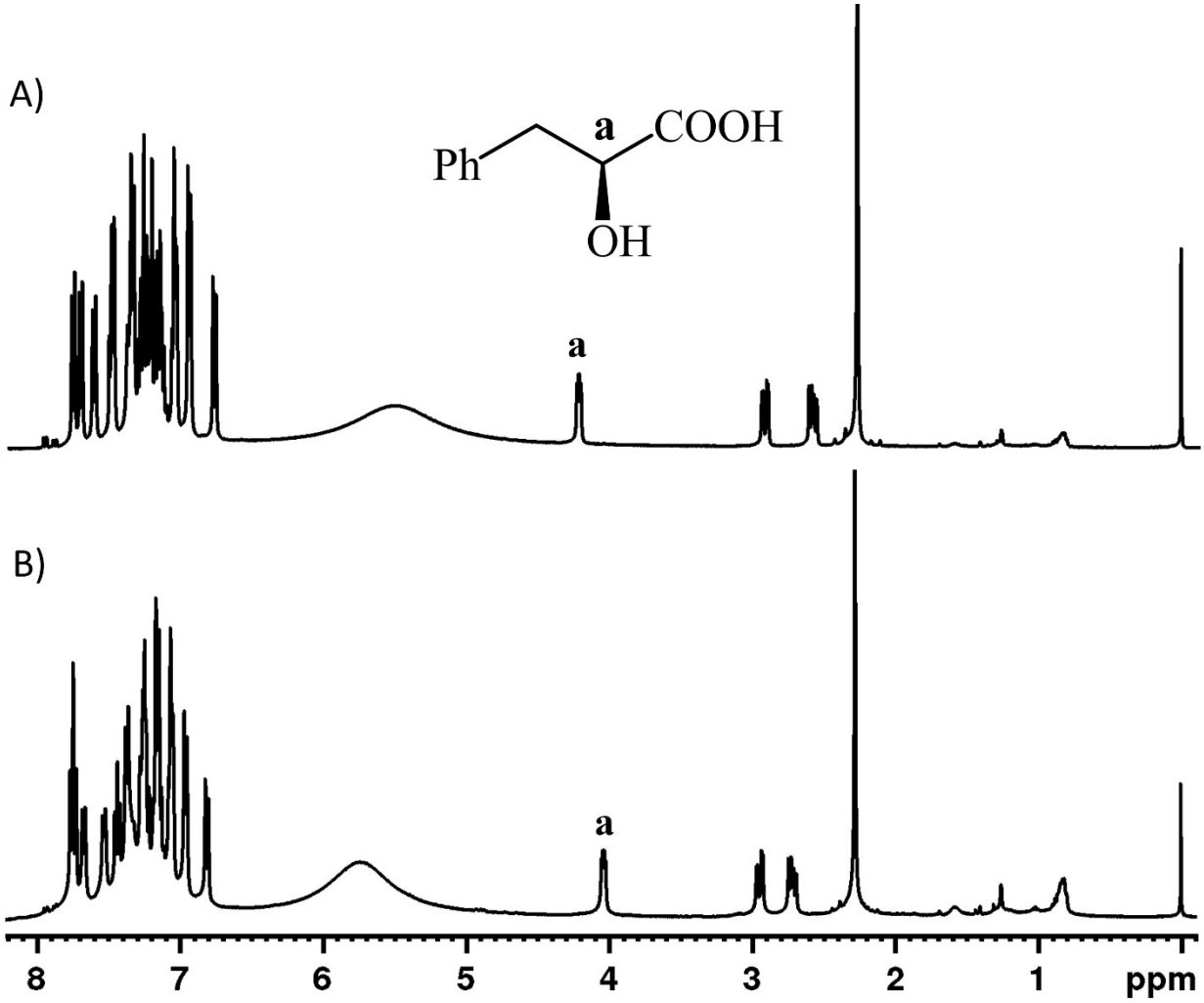
400 MHz ^{1}H-NMR spectra of (*R*) -Mandelic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN



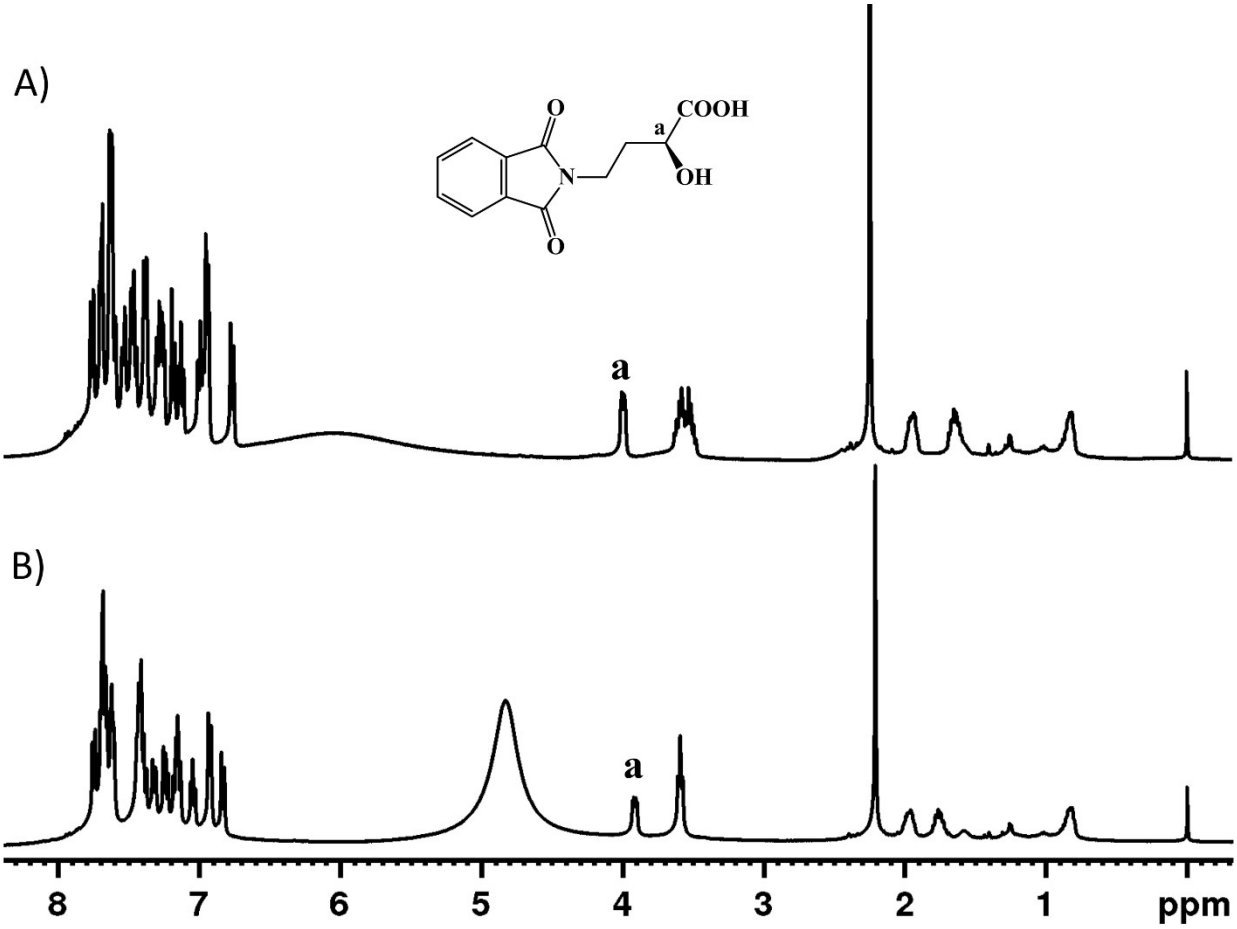
400 MHz ^{1}H-NMR spectra of (*S*) -Mandelic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN



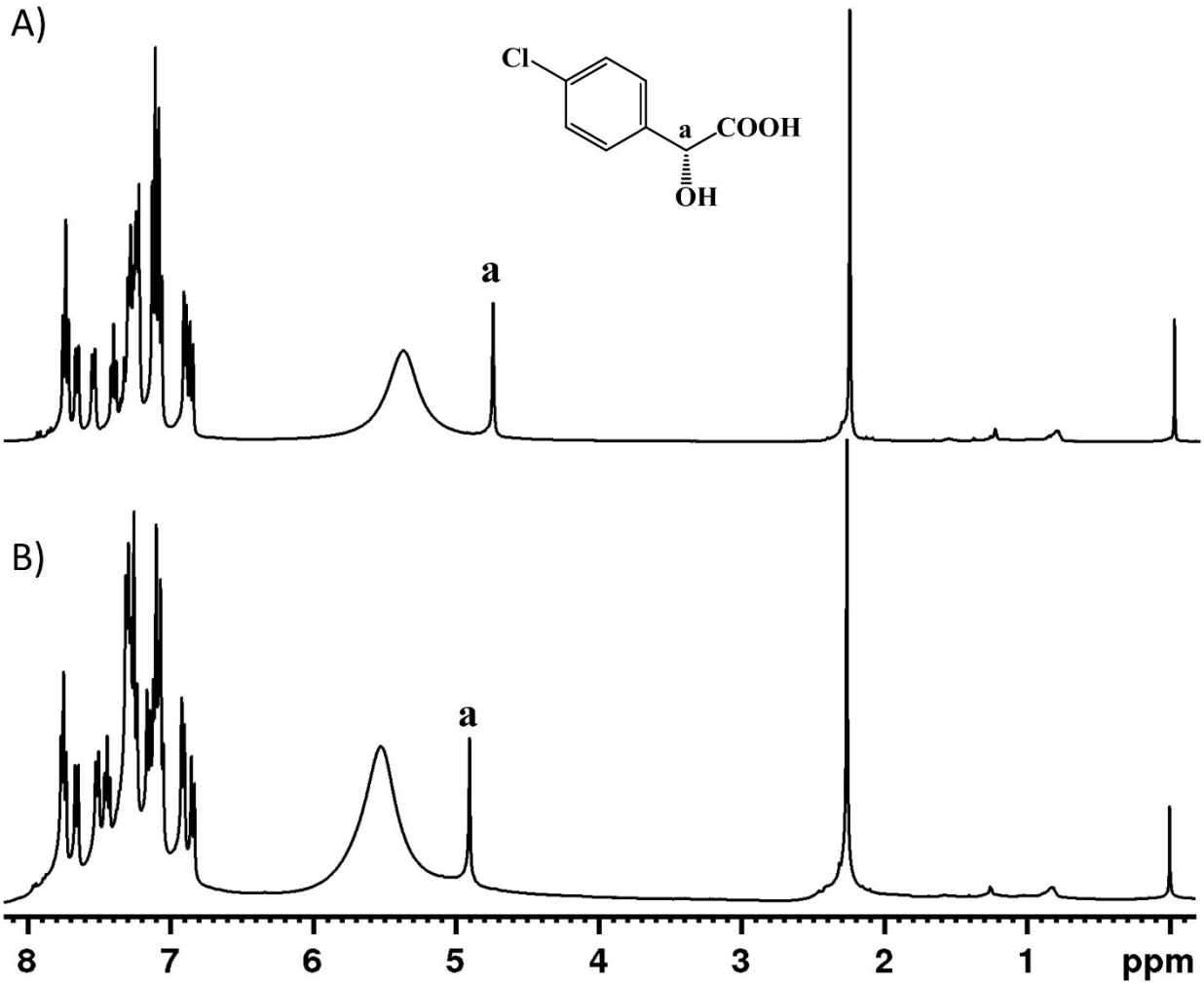
400 MHz ^{1}H-NMR spectra of (*L*) -Phenyl lactic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN



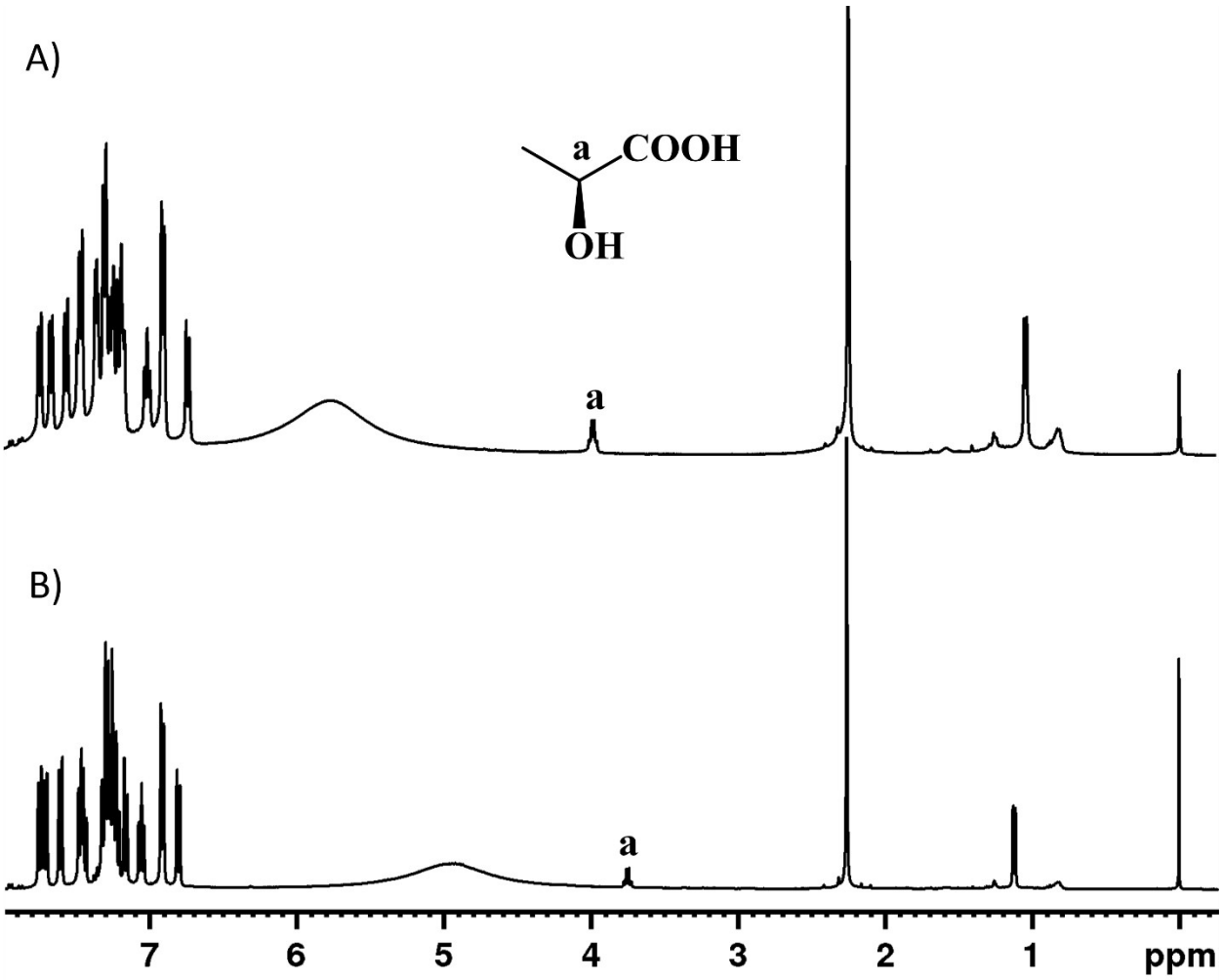
400 MHz ^{1}H-NMR spectra of (*2S*)-4-(1, 3-Dioxoisoindolin-2-yl)-2-hydroxybutanoic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN



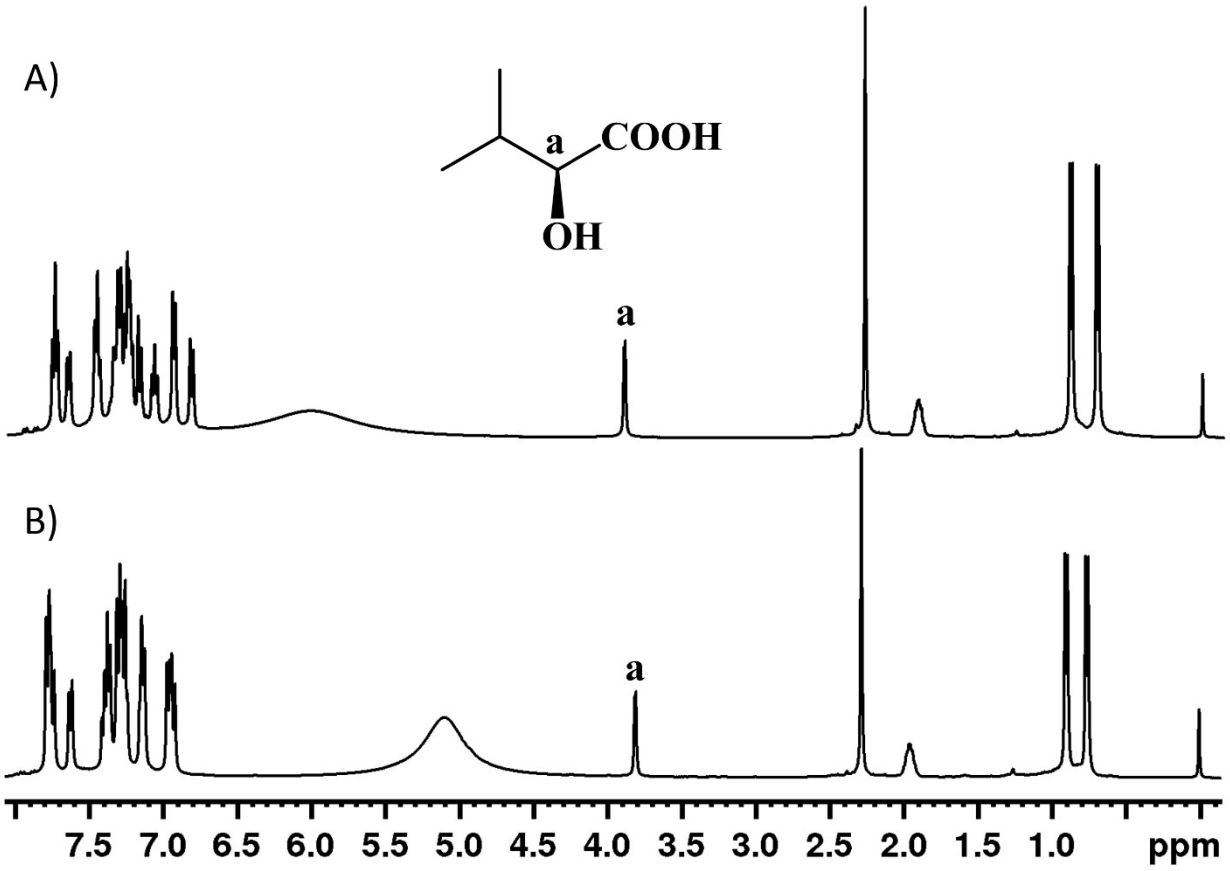
400 MHz ^{1}H-NMR spectra of (*R*)-4-Chloromandelic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN



400 MHz ^{1}H-NMR spectra of (*L*) -Lactic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN

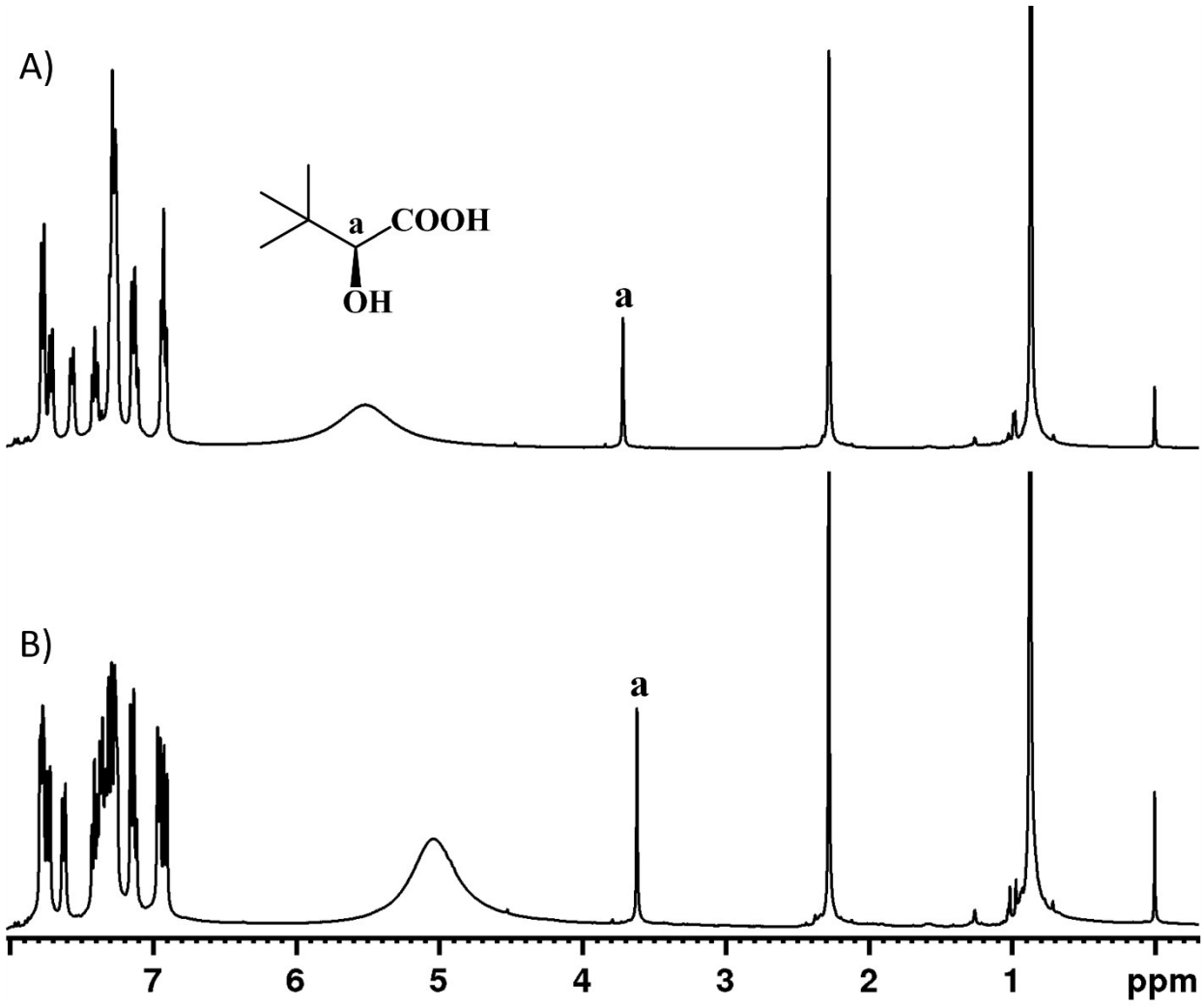


400 MHz ^{1}H-NMR spectra of (*S*)-2-Hydroxy-3-methyl butyric acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN



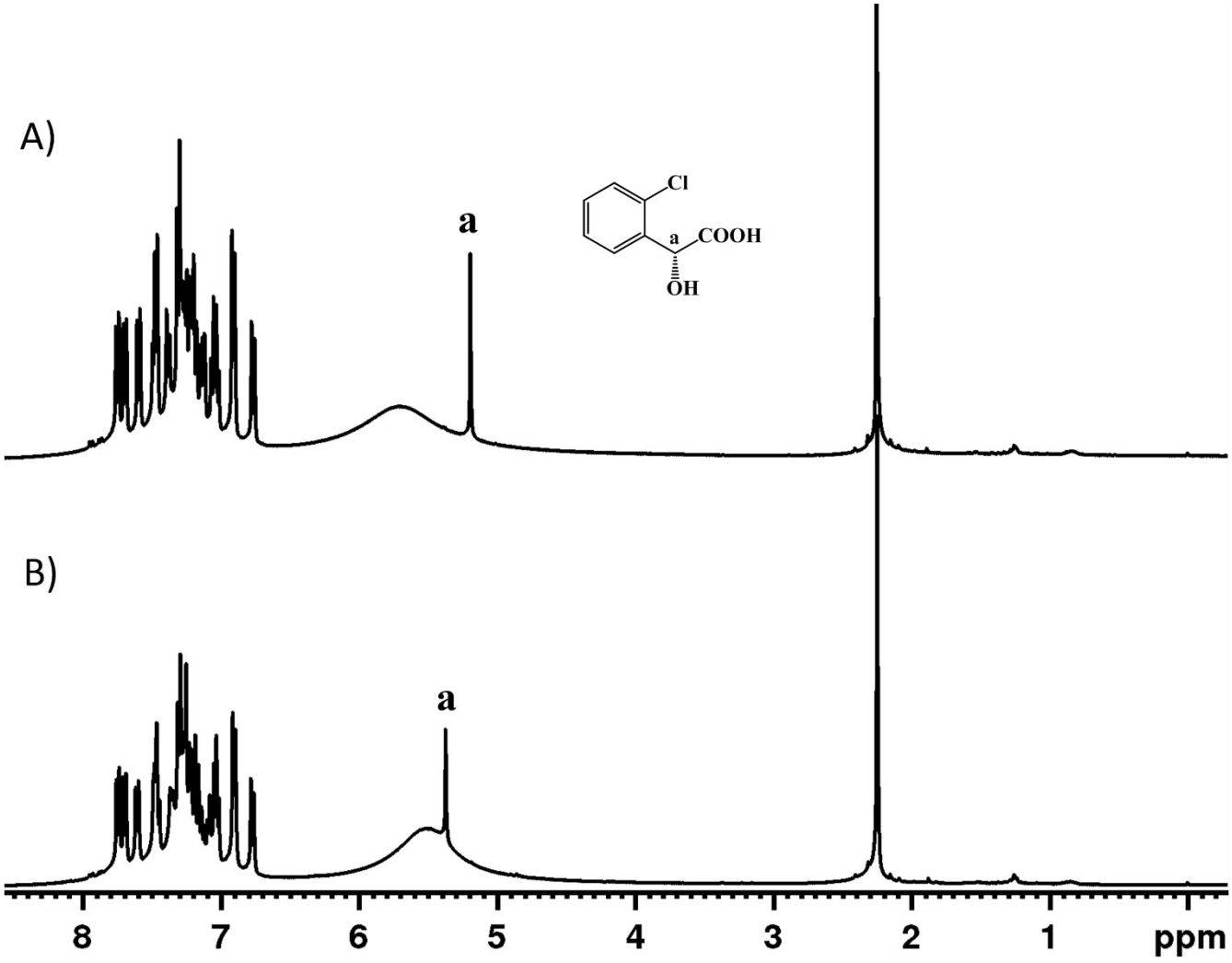
S54

400 MHz ^{1}H-NMR spectra of (*S*) -2-Hydroxy-3, 3-dimethyl butyric acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN

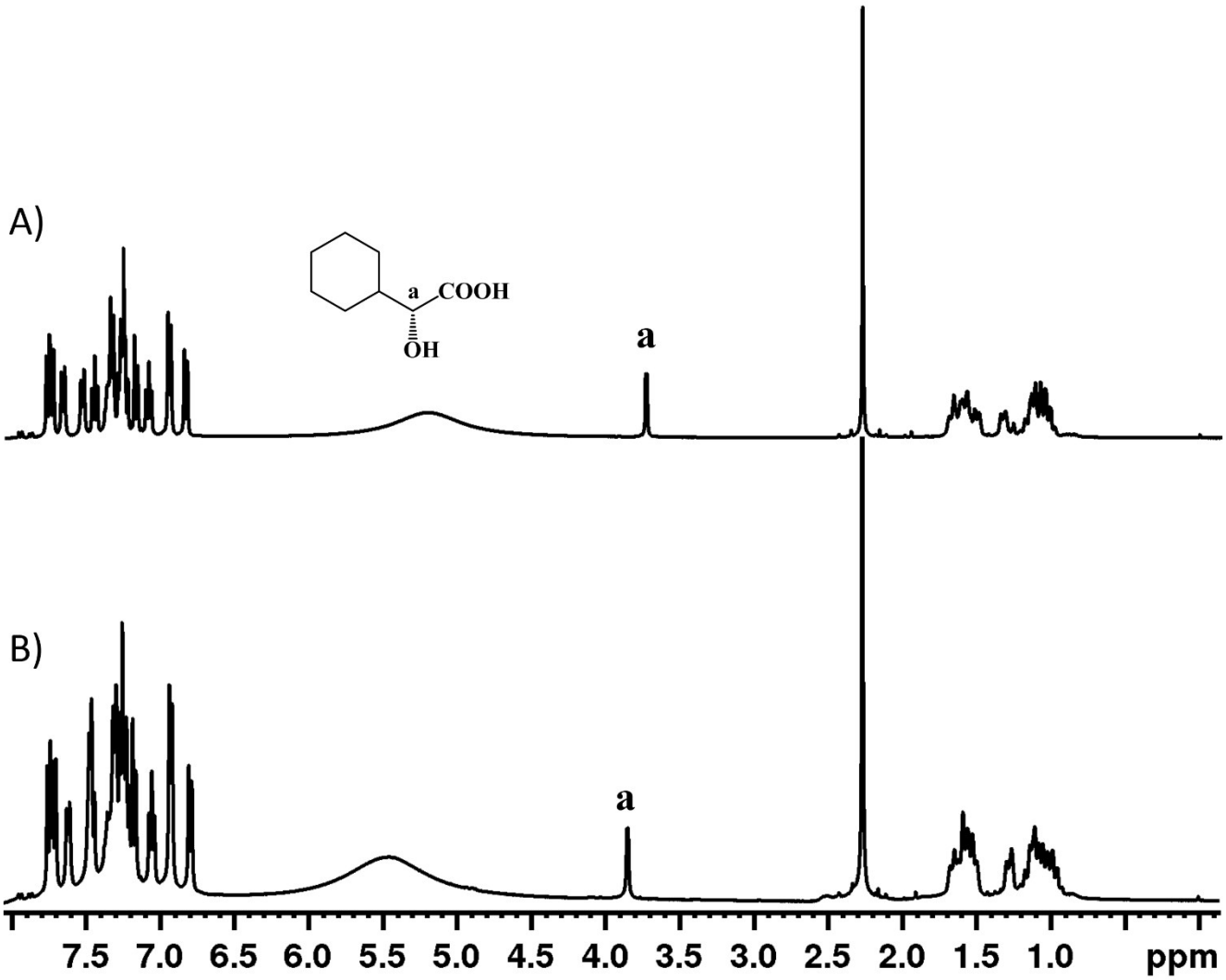


S55

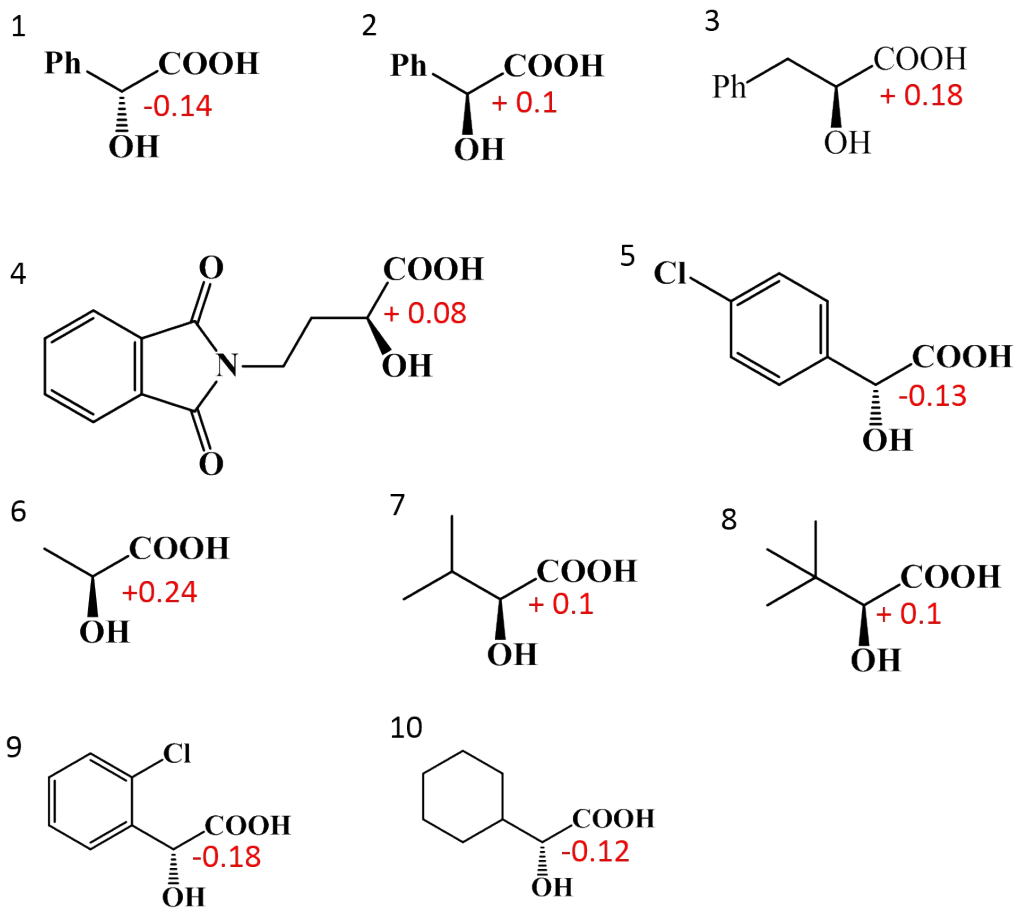
400 MHz ^{1}H-NMR spectra of (*R*) -2-Chloro mandelic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN



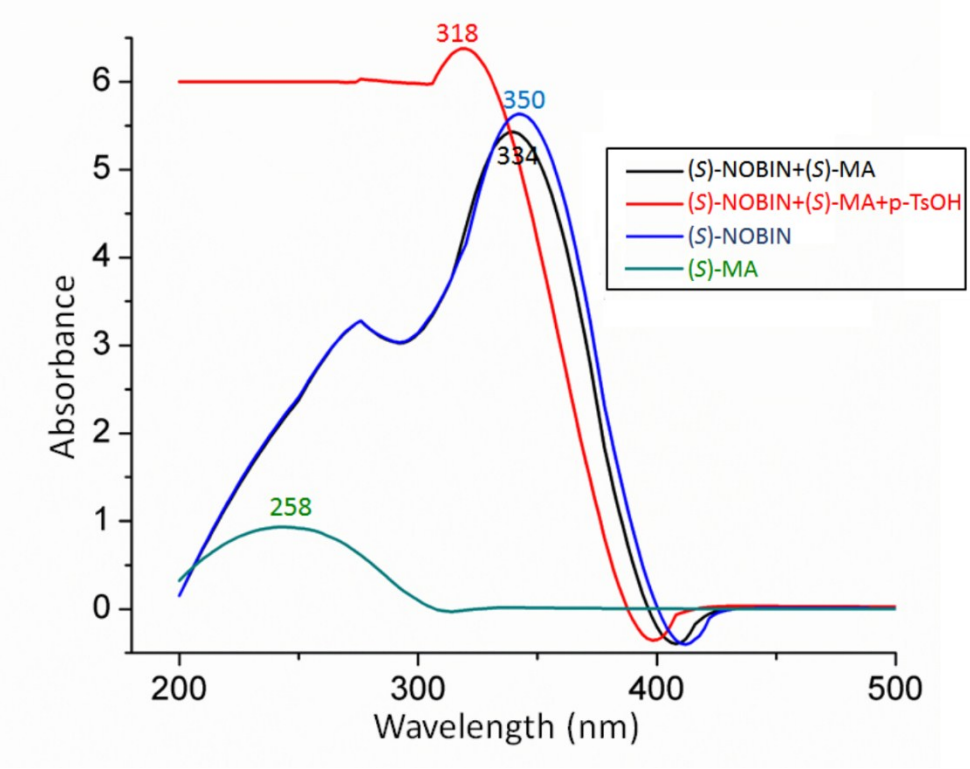
400 MHz ^{1}H-NMR spectra of (*R*)-Hexahydromandelic acid and p-TsOH in presence of A) (*R*)-NOBIN and B) (*S*)-NOBIN



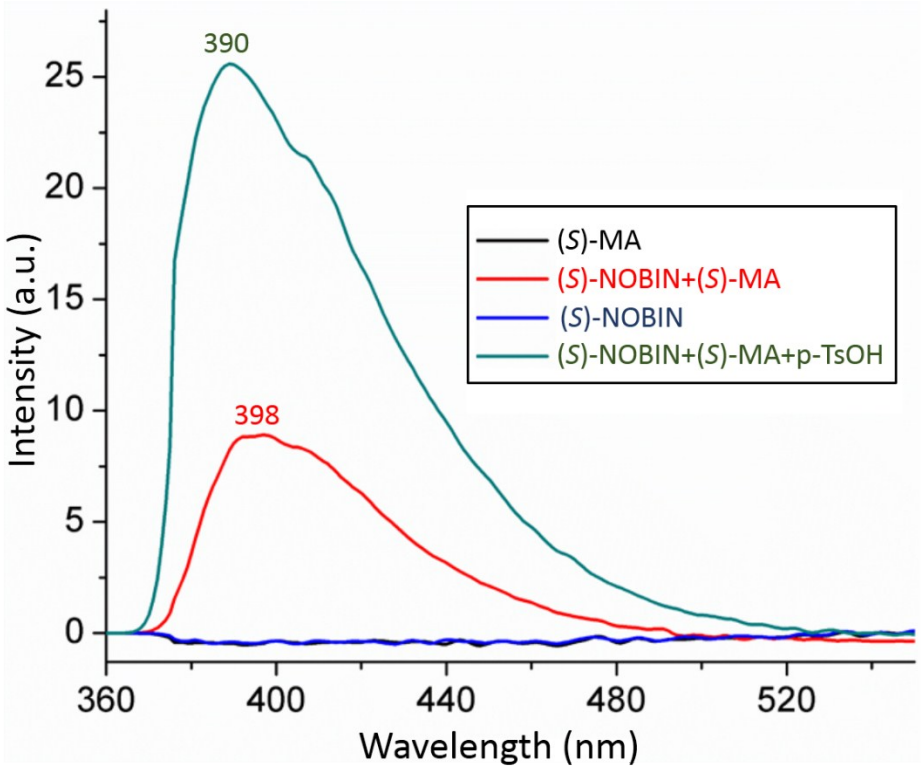
Molecular structure with $\Delta\delta^{R,S}$ values for alpha proton



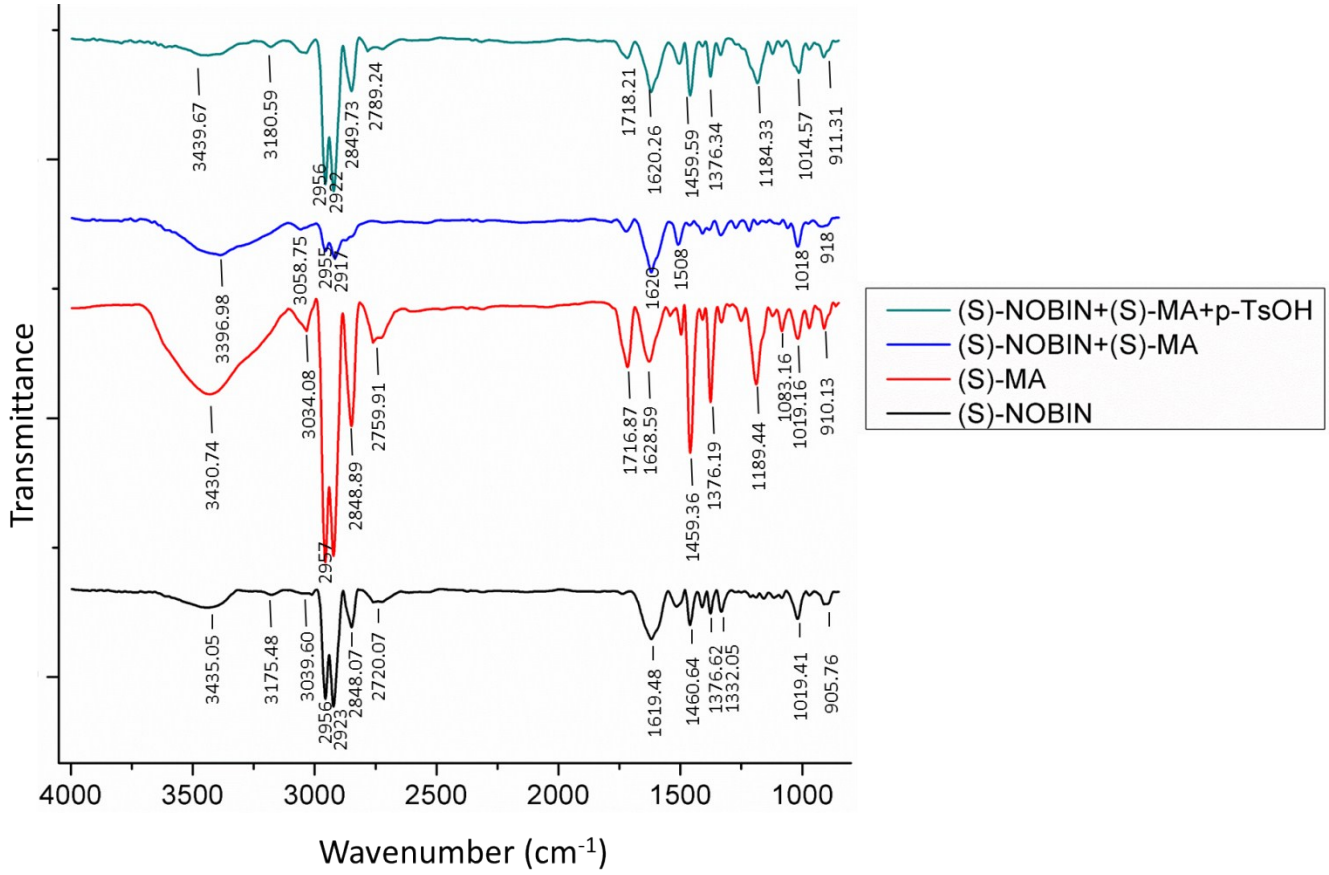
UV-Vis Spectra ($CHCl_3$ solvent)



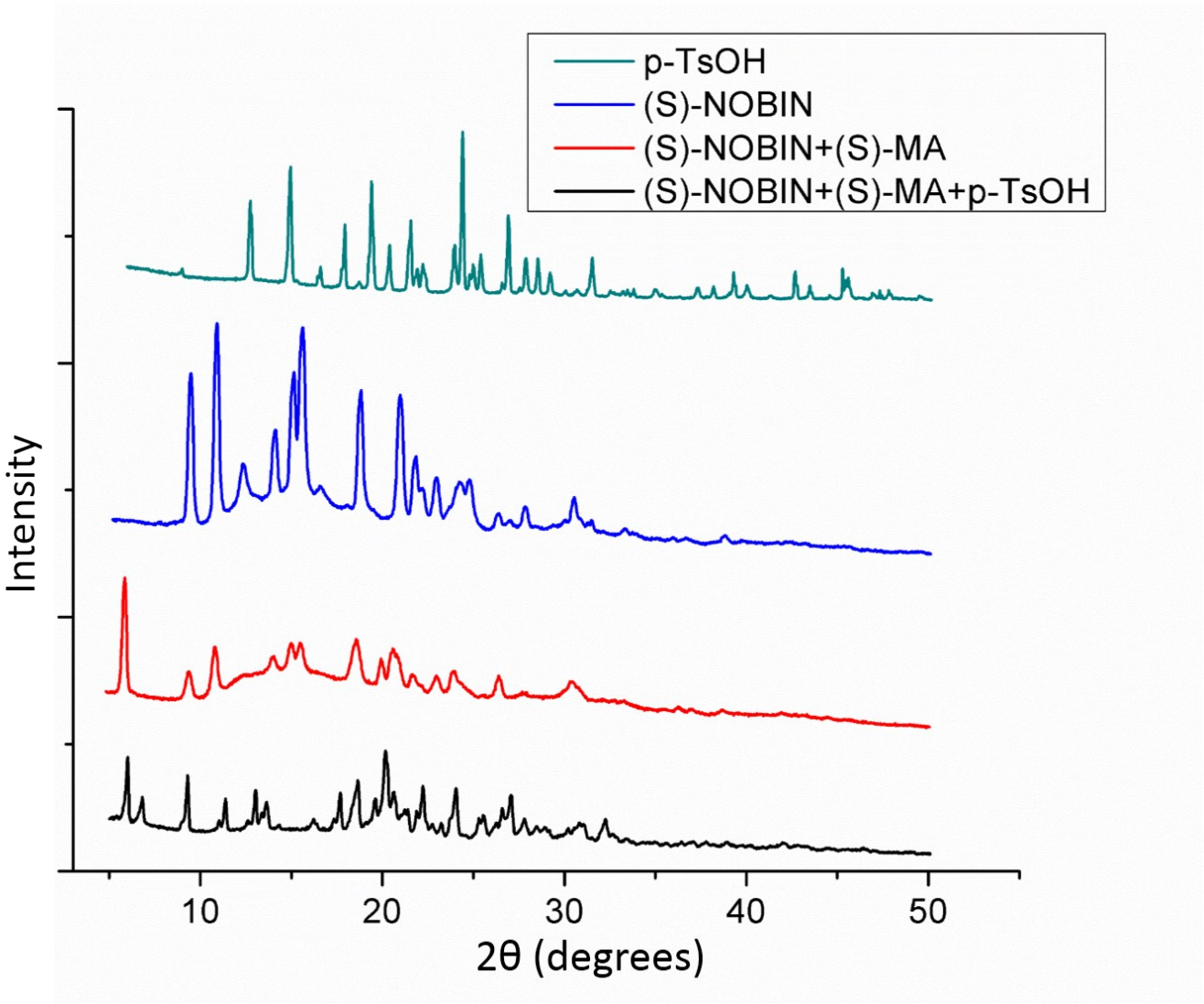
Fluorescence Spectra ($CHCl_3$ solvent)



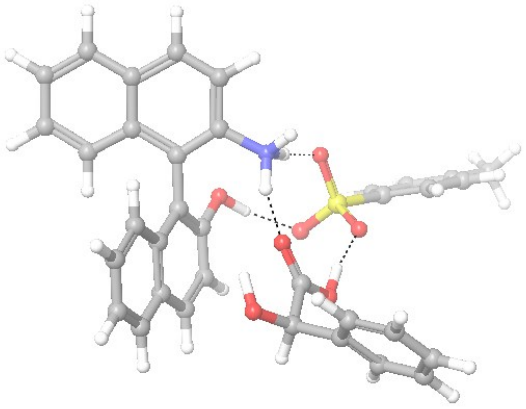
IR Spectra ($CHCl_3$ solvent)



PXRD patterns



Coordinates for (*R*)-NOBIN/ (*R*)-Mandelic acid/ p-TsOH complex (Gaussian 09)



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C	3.58437600	2.27713300	-2.36265400
C	4.64834400	2.60719200	-1.55527600
C	4.93690100	1.81284300	-0.42240800
C	4.17527800	0.70271600	-0.12530400
C	2.25737100	-0.82170600	-0.67414900
H	3.33837300	2.88907400	-3.22643000
H	5.25502800	3.47989700	-1.77503800
H	5.76726400	2.08152400	0.22437500
H	4.41170100	0.10747300	0.74979200
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C	1.16434000	-1.09545500	-1.49383800
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C	3.88191100	-3.42179300	1.68227900

C	2.93543000	-3.41821300	2.73852800
C	1.81905200	-2.62365700	2.66946900
C	1.62479400	-1.78472300	1.55111800
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C	5.70059800	-3.46835600	-0.45844400
C	5.92316800	-4.28074500	0.67829900
C	5.02962400	-4.25824500	1.72310300
H	3.09794400	-4.06079200	3.59865200
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H	6.40067100	-3.50188000	-1.28774000
H	6.79488800	-4.92688100	0.71841300
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H	-0.45823900	-1.52166100	1.13467300
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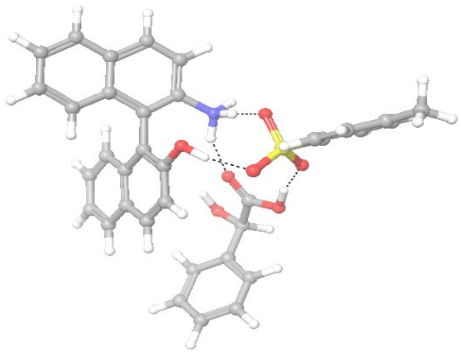
Coordinates for (*S*)-NOBIN/ (*R*)-Mandelic acid/ p-TsOH complex (Gaussian 09)



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C	-5.44903300	1.05489000	-0.16012500
C	-5.29872600	-0.16265300	0.54237500
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H	-2.58991700	-6.98854100	0.75172500
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C	4.86793200	-0.19776200	-0.17012600
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H	9.39538400	-0.74908000	-1.74447700
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C	-0.78614700	5.90259900	-1.20989500
C	-2.11689000	6.00968500	-1.61989300
C	-3.11209200	5.34900000	-0.89945100
C	-2.78071000	4.58072600	0.21906100
C	-1.11221700	3.64458200	1.88247200
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H	-2.37492400	6.60890000	-2.48842300
H	-4.15234800	5.43742700	-1.20154100
H	-3.54749800	4.07279800	0.79171000
C	-0.13971700	2.49825700	1.56797400
H	-0.60007100	4.30316100	2.59687000
O	-2.25309700	3.11613800	2.51510500
O	1.07356800	2.89657500	1.28709700
O	-0.52902600	1.33150700	1.61201200
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H	1.71952000	2.13790200	1.09725700
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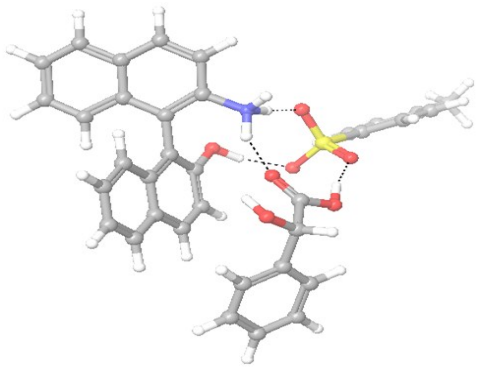
Coordinates for (*R*)-NOBIN/ (*S*)-mandelic acid/ p-TsOH complex (Gaussian 09)



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C	4.13943200	0.88590100	-0.43962400
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H	6.10845600	0.50544300	-1.17119300
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C	2.11142200	-1.29399800	1.83462900
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H	0.10408800	-0.97216500	2.51802900
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H	4.63397200	4.84986600	2.38780600
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H	-1.12292200	0.80507700	1.55803700
H	0.28818500	0.50308300	-1.33497700
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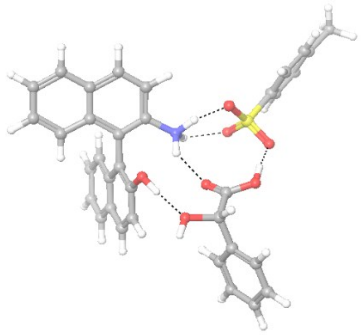
H	-1.72465300	-2.13088400	-1.09723300
H	-0.30508900	1.38604500	-2.58578000

Coordinates for (*S*)-NOBIN/ (*S*)-mandelic acid/ p-TsOH complex (Gaussian 09)



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C	-4.17690200	-1.80667300	3.44624300
C	-3.63441900	-1.73645200	2.18185200
C	-2.85589400	-0.37067700	0.22429900
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H	-4.31965800	-2.77626400	3.91448600
H	-3.35456200	-2.64853800	1.66747800
C	-3.54357200	1.96959200	1.65967500
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C	-2.47675200	-1.58304100	-0.56766900
H	-3.81203200	2.86828600	2.20862800
H	-2.76993700	3.03357600	-0.03374000
O	-2.04151400	0.98600300	-1.52933200
C	-3.47188100	-2.48696800	-1.07611400
C	-3.06619400	-3.66847000	-1.78243500

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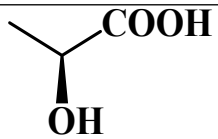
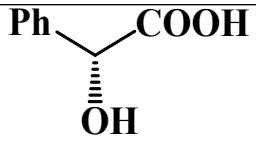
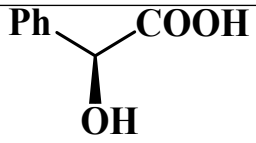
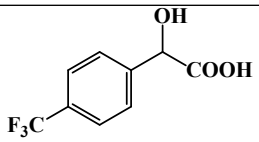
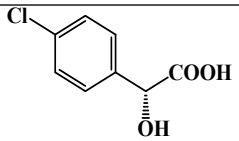
Comparison of the present protocol with other protocols reported in the literature (Alpha proton)

	1) +0.24 2) - 0.07 3) -0.01	1) Present method 2) Freire, F.; Quiñoá, E.; Riguera, R. Chem. Commun. (Camb). 2008, 35, 4147. 3) Chaudhari, S. R.; Suryaprakash, N. New J. Chem.2013, 37, 4025
	1) -0.12 2) +0.03	1) Present method 2) Chaudhari, S. R.; Suryaprakash, N. New J. Chem.2013, 37, 4025.
	1) +0.14 2) -0.03 3) -0.04	1) Present method 2) Chaudhari, S. R.; Suryaprakash, N. New J. Chem.2013, 37, 4025 3) Freire, F.; Quiñoá, E.; Riguera, R. Chem. Commun. (Camb). 2008, 35, 4147.
	1) 0.24 2) 0.1	1) Present method 2) Chaudhari, S. R.; Suryaprakash, N. New J. Chem.2013, 37, 4025
	1) -0.13	1) Present method 2) Chaudhari, S. R.; Suryaprakash, N.

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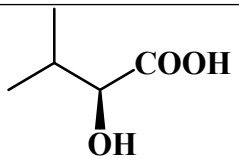
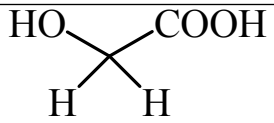
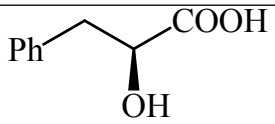
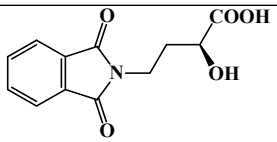
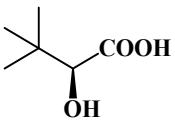
	1) +0.1 2) - 0.03 3) -0.12	1) Present method 2) Chaudhari, S. R.; Suryaprakash, N. New J. Chem.2013, 37, 4025 3) Freire, F.; Quiñoá, E.; Riguera, R. Chem. Commun. (Camb). 2008, 35, 4147.
	1) 0.19 2) 0.08	1) Present method 2) Freire, F.; Quiñoá, E.; Riguera, R. Chem. Commun. (Camb). 2008, 35, 4147.
	1) +0.18 2) -0.02	1) Present method 2) Chaudhari, S. R.; Suryaprakash, N. New J. Chem.2013, 37, 4025
	1) +0.09 2) -0.02	1)Present method 2) Chaudhari, S. R.; Suryaprakash, N. New J. Chem.2013, 37, 4025.
	1) +0.1 2) -0.03	1) Present method 2) Chaudhari, S. R.; Suryaprakash, N. New J. Chem.2013, 37, 4025

Reference

Gaussian 09, Revision D.01,M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Menucci,G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H.Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.