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SUPPORTING INFORMATION

A Simple and Rapid Approach for Testing Enantiopurity of Hydroxy acids and their Derivatives using ^{1}H NMR Spectroscopy

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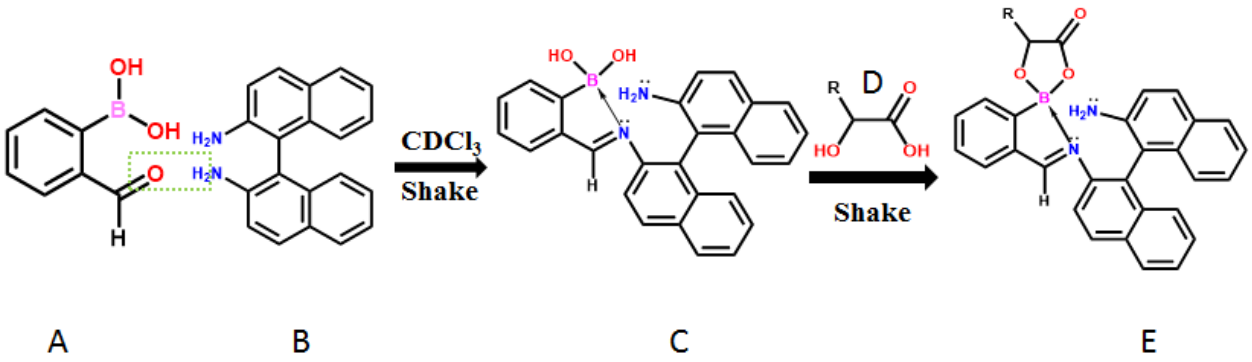
Contents

(a) Mandelic acid (b) 2-Cl-mandelic acid (c) 4-Br--mandelic acid (d) 4-trifluoromethyl mandelic acid (e) 3,4-(Methylenedioxy)mandelic acid (f) 2-hydroxy-3-methyl butyric acid (g) Methyl-2,3-dihydroxy-3-phenyl propionate (h) Malic acid

Scheme.



Scheme.1S: The stepwise general scheme for the coupling reaction.

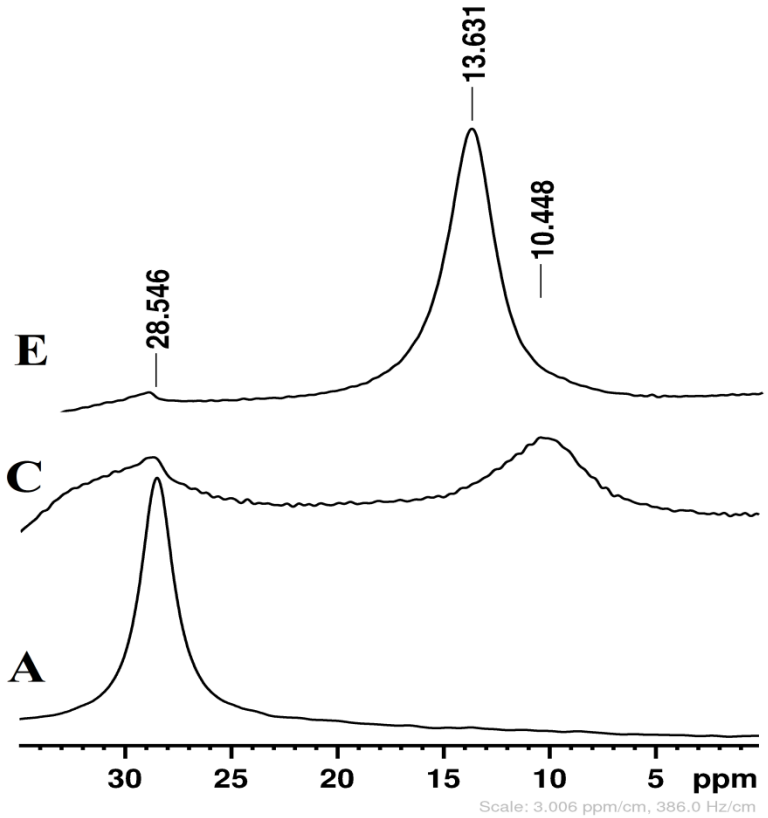


Fig.1S. ^{11}B NMR spectra of (A) 2-formylphenyl boronic acid (C) Amino-binaphthalene-benzoazaborole complex and (E) Iminoboronate ester complex with mandelic acid acquired on 400 MHz NMR spectrometer.

In the ^{11}B NMR spectrum of 2-formylphenylboronic acid a peak was detected at 28.55 ppm. The dishielding is due to the electron deficiency of three-coordinated Boron atom. On complexation with [1,1-binaphthaline]-2,2-diamine boron atom become tetra-coordinated. As a consequence the peak in ^{11}B NMR spectrum is shifted to 10.45 ppm. Again on complexation with the acid some change in the electronic environment is observed and the ^{11}B NMR peak appeared at 13.63 ppm.

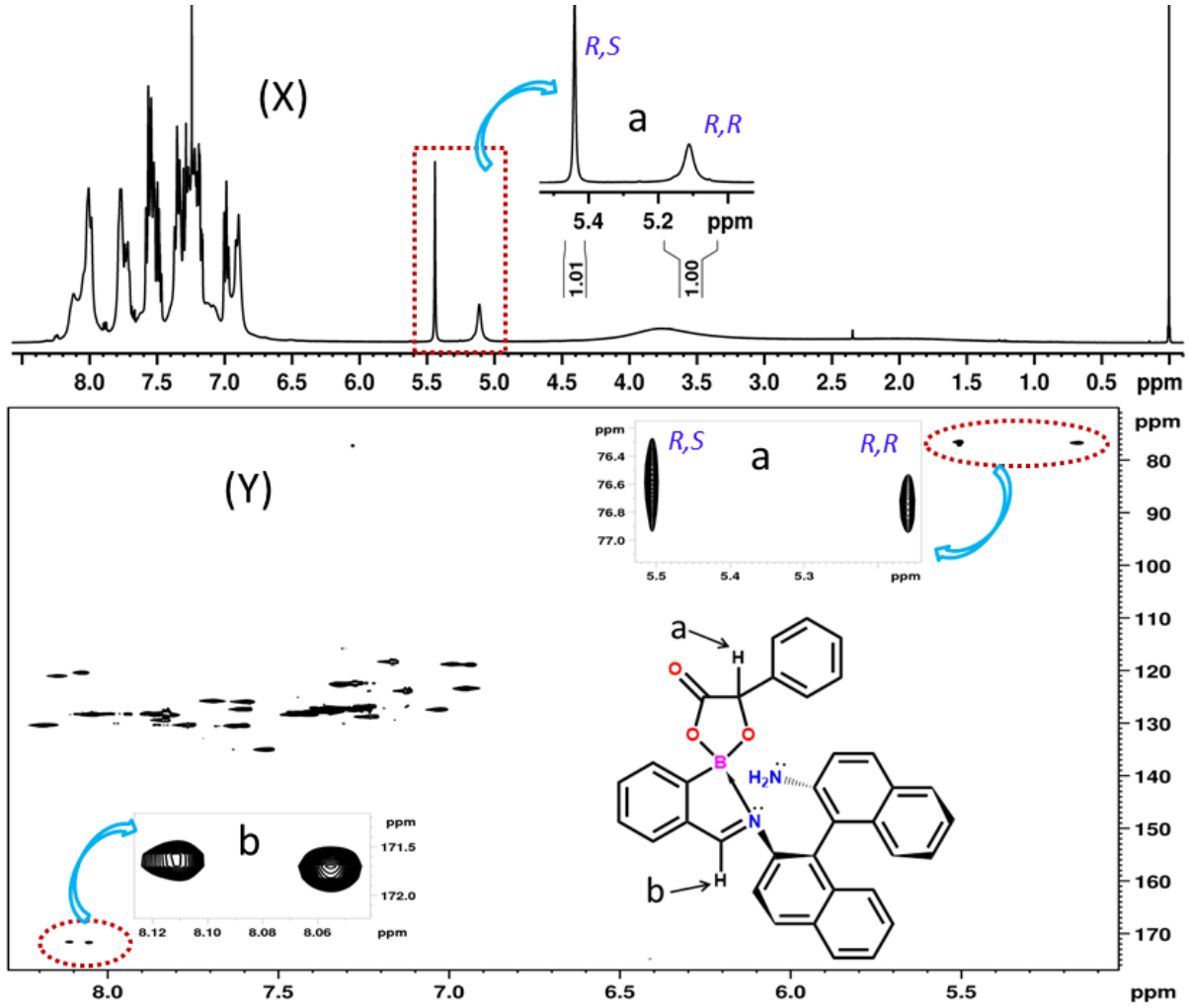


Fig.2S. 400 MHz (X) ^{1}H and (Y) ^{1}H-^{13}C-HSQC NMR spectrum of *R/S*-Mandelic acid in iminoboronate complex E. The discriminated peaks are marked inside the dotted circle and expanded region is given as an inset.

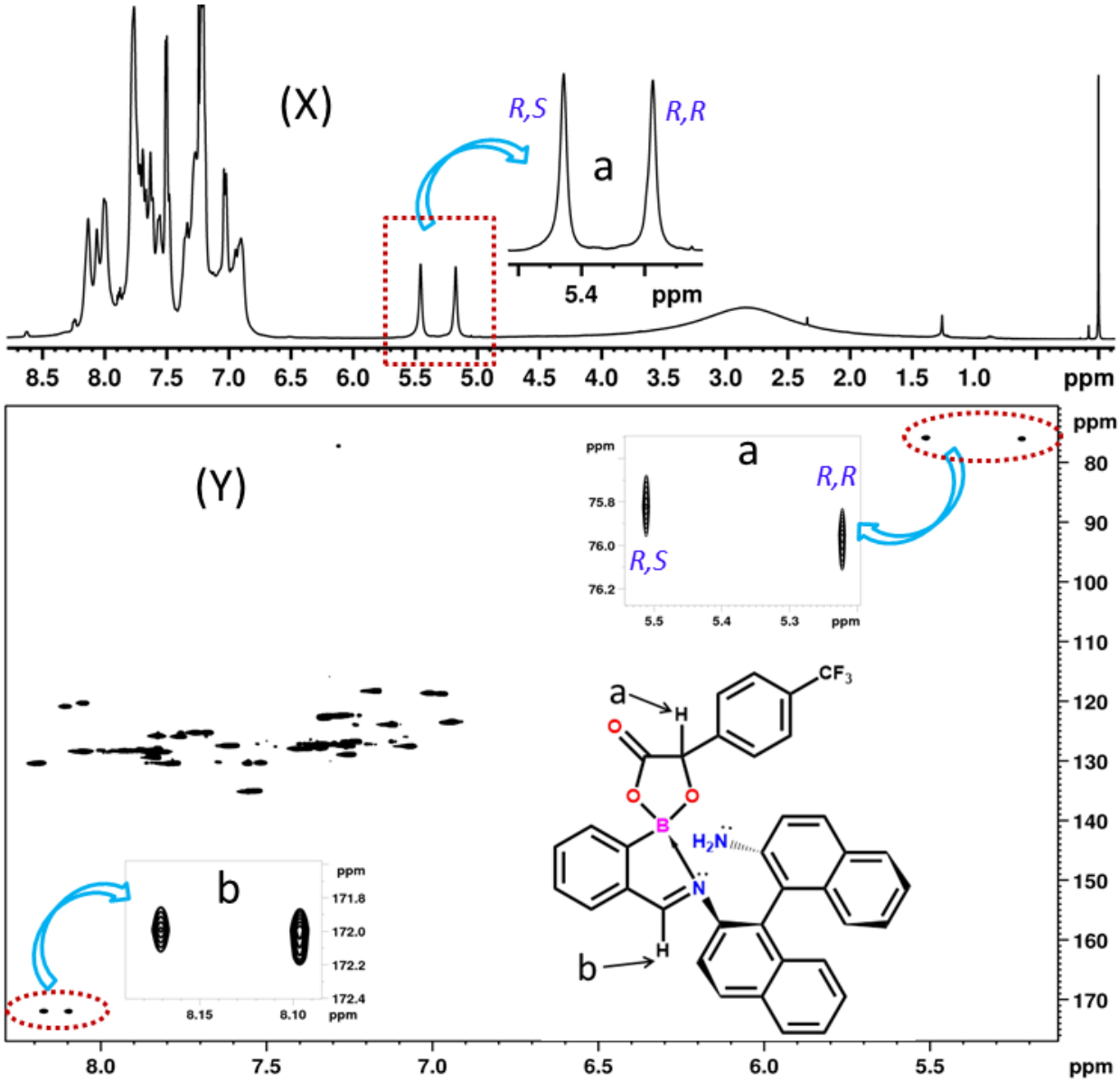


Fig.3S. 400 MHz (X) ^{1}H and (Y) ^{1}H-^{13}C-HSQC NMR spectrum of *R/S*-4-trifluoromethyl Mandelic acid in iminoboronate complex E. The discriminated peaks are marked inside the dotted circle and expanded region is given as an inset.

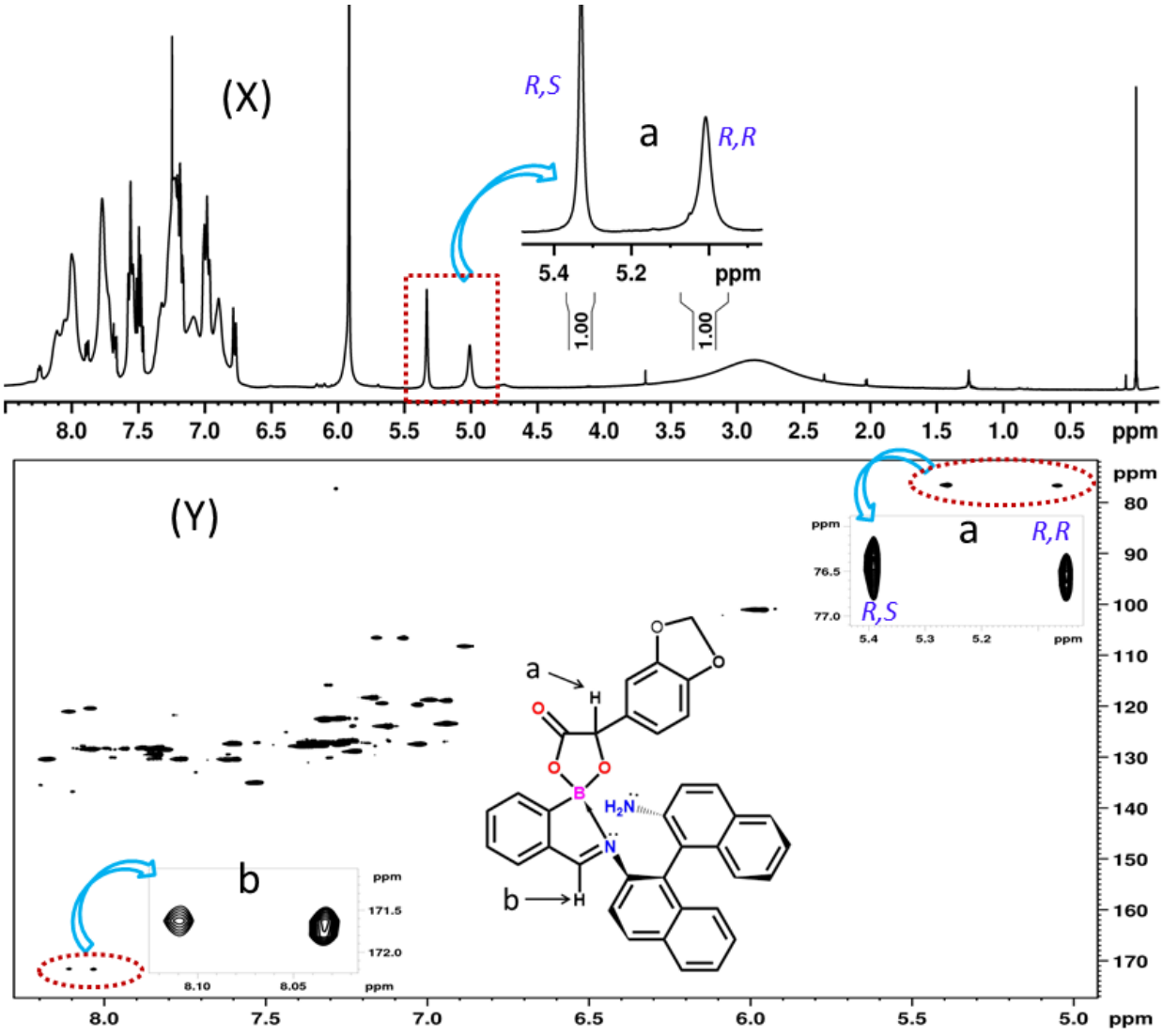


Fig.4S. 400 MHz (X) ^{1}H and (Y) ^{1}H-^{13}C-HSQC NMR spectrum of *R/S*-3,4-(Methylenedioxy)mandelic acid in iminoboronate complex E. The discriminated peaks are marked inside the dotted circle and expanded region is given as an inset.

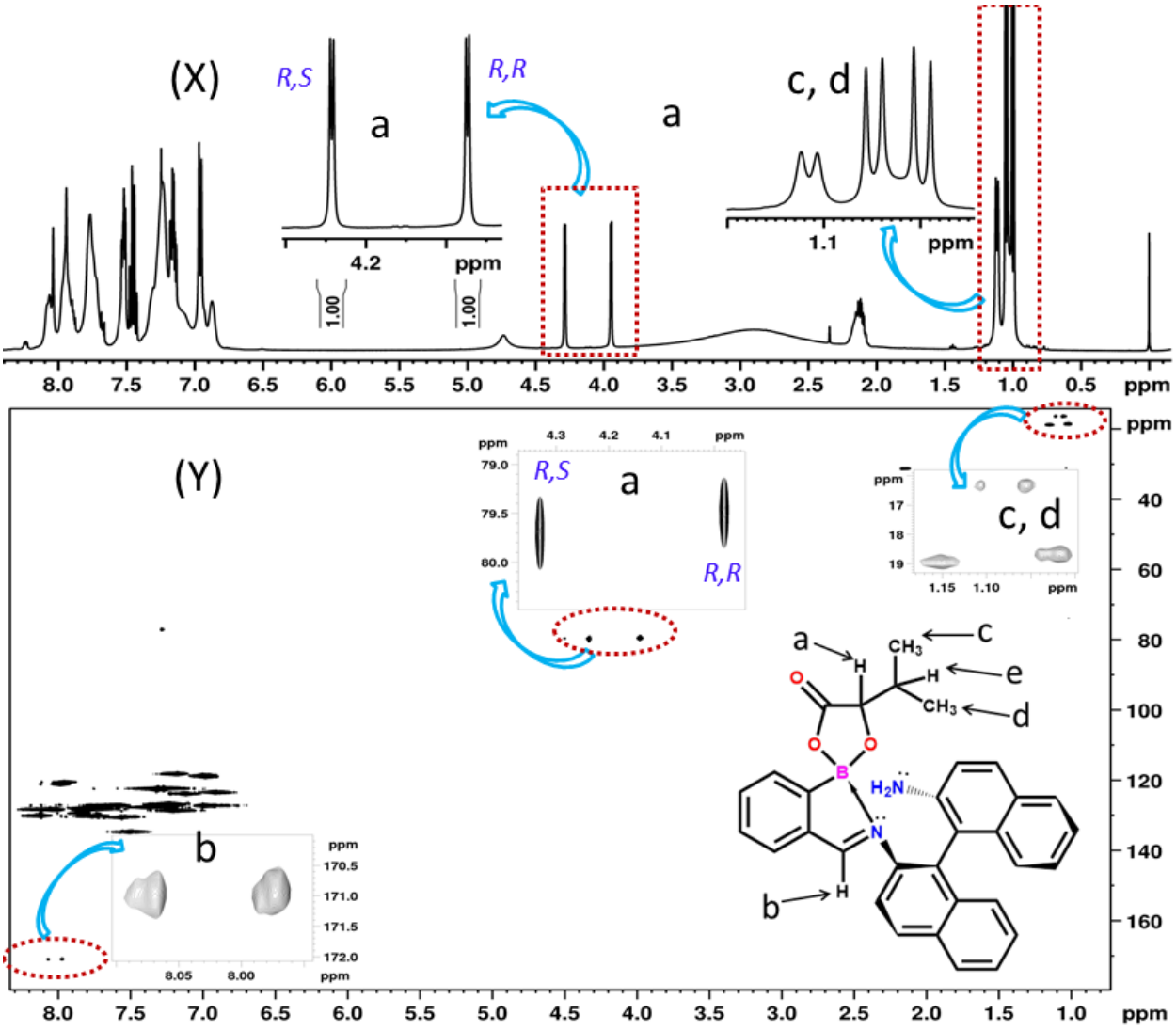


Fig.5S. 400 MHz (X) ^{1}H and (Y) ^{1}H-^{13}C-HSQC NMR spectra of *R/S*-2-hydroxy-3-methyl-butyric acid in the iminoboronate complex E. The discriminated peaks are marked inside the dotted circle and expanded region is given as an inset.

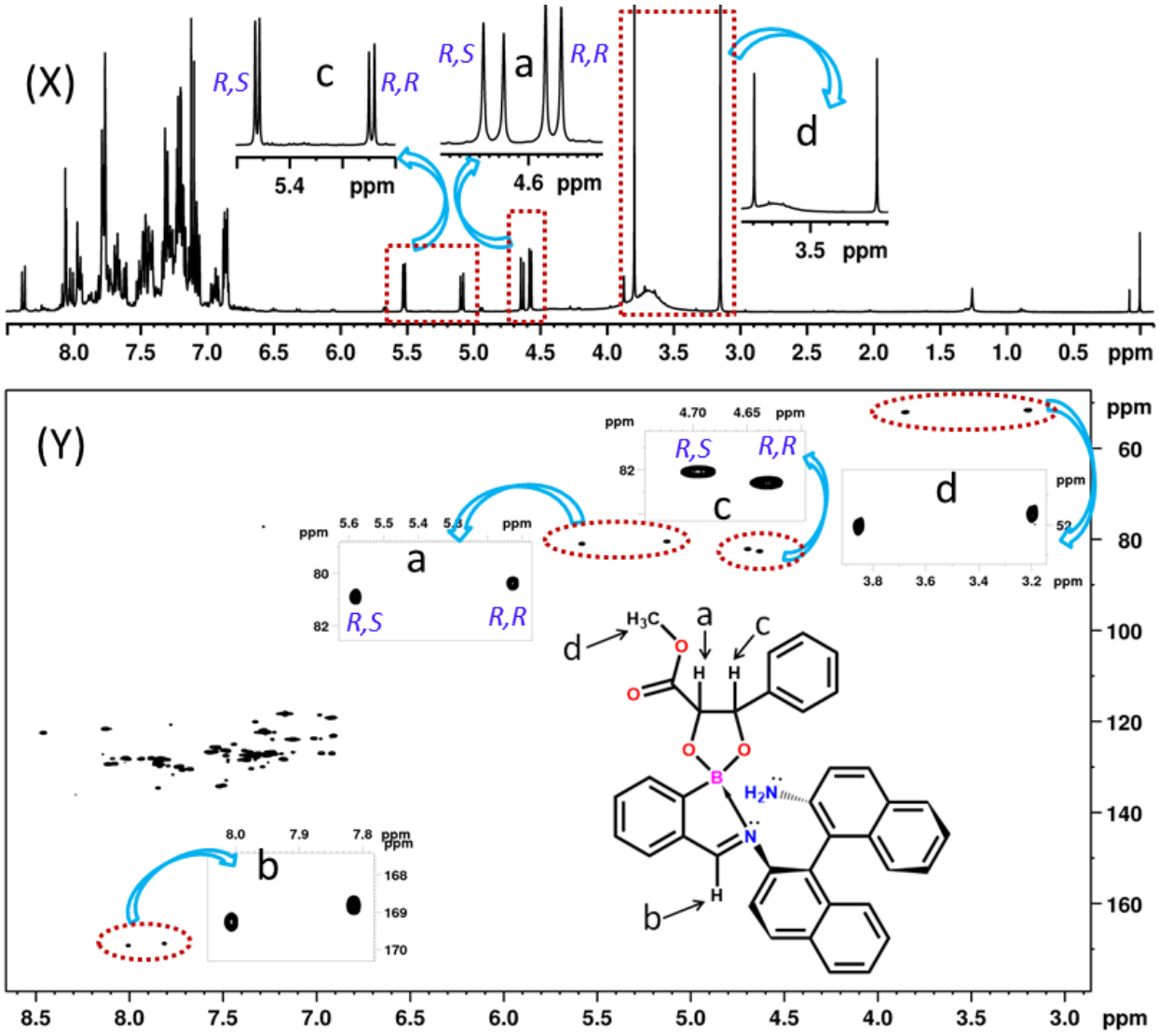


Fig.6S. 400 MHz (X) ^{1}H and (Y) ^{1}H-^{13}C-HSQC NMR spectra of *R/S*-Methyl-2,3-dihydroxy-3-phenyl propionate in the iminoboronate complex E. The discriminated peaks are marked inside the dotted circle and expanded region is given as an inset.

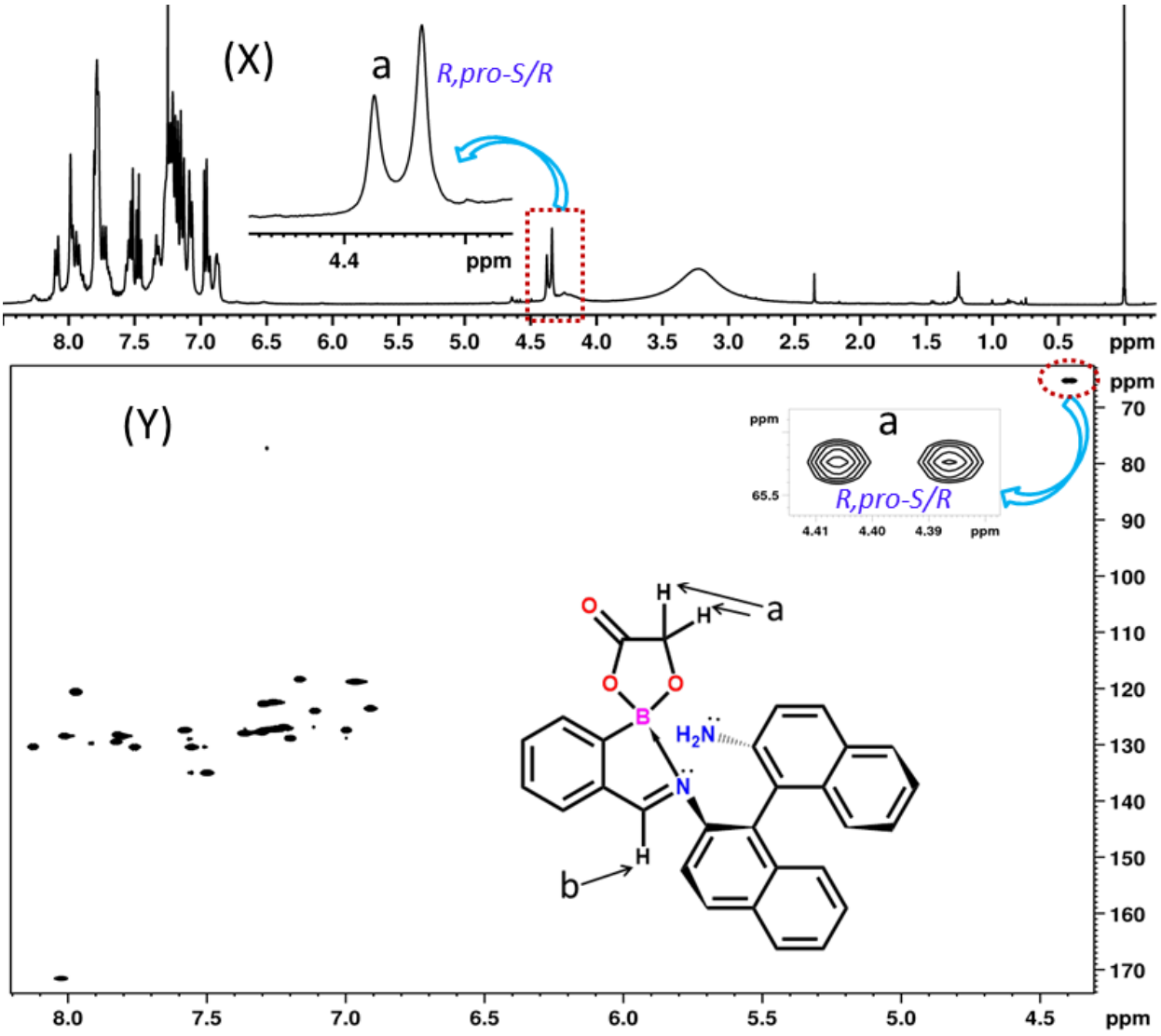
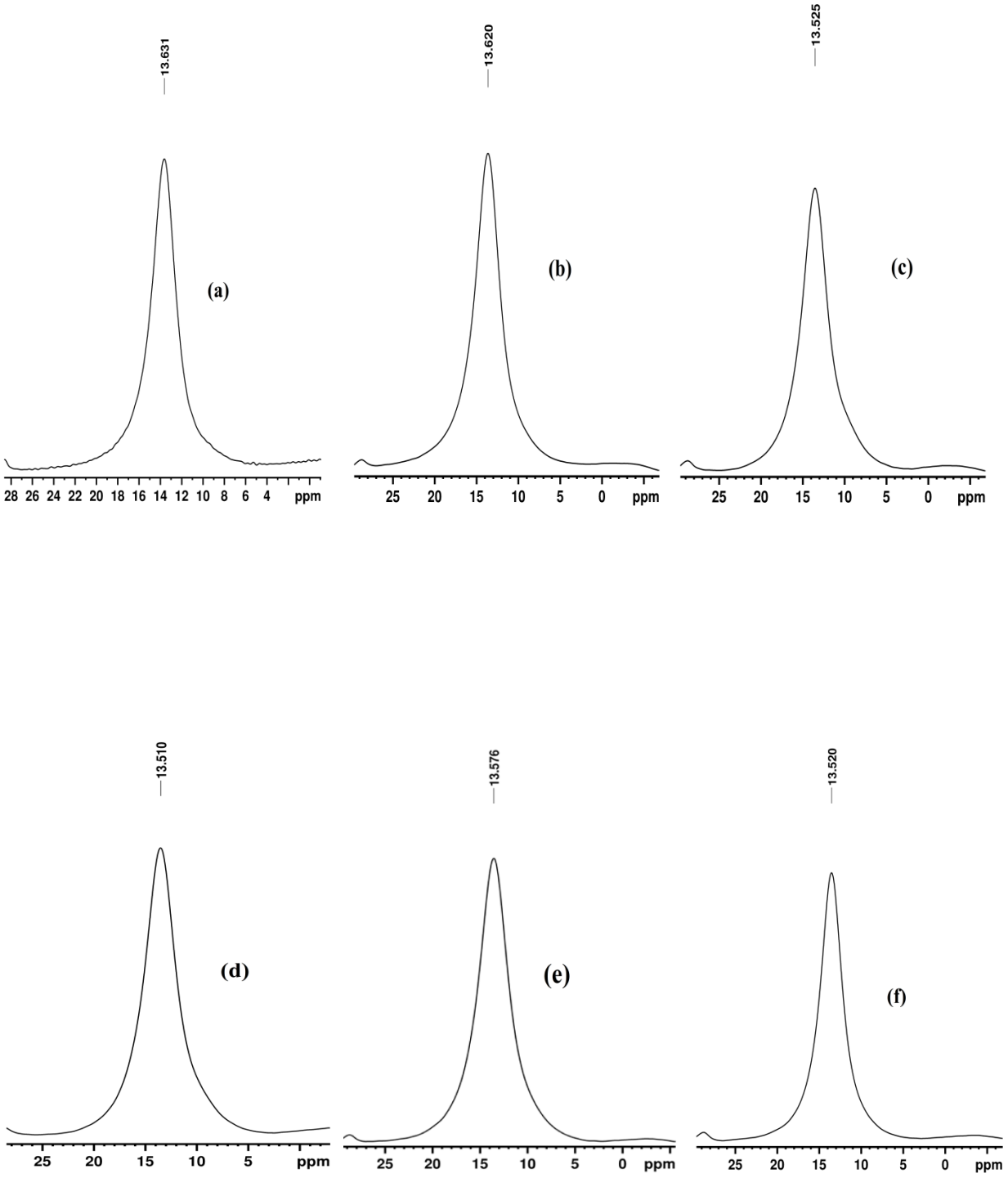


Fig.7S. 400 MHz (X) ^{1}H and (Y) ^{1}H-^{13}C-HSQC NMR spectra of *R/S*-Glyconic acid in the iminoboronate complex E. The discriminated peaks are marked inside the dotted circle and expanded region is given as an inset.


13.631
(a)
28 26 24 22 20 18 16 14 12 10 8 6 4 ppm
13.620
(b)
25 20 15 10 5 0 ppm
13.525
(c)
25 20 15 10 5 0 ppm
13.510
(d)
25 20 15 10 5 ppm
13.576
(e)
25 20 15 10 5 0 ppm
13.520
(f)
25 20 15 10 5 0 ppm

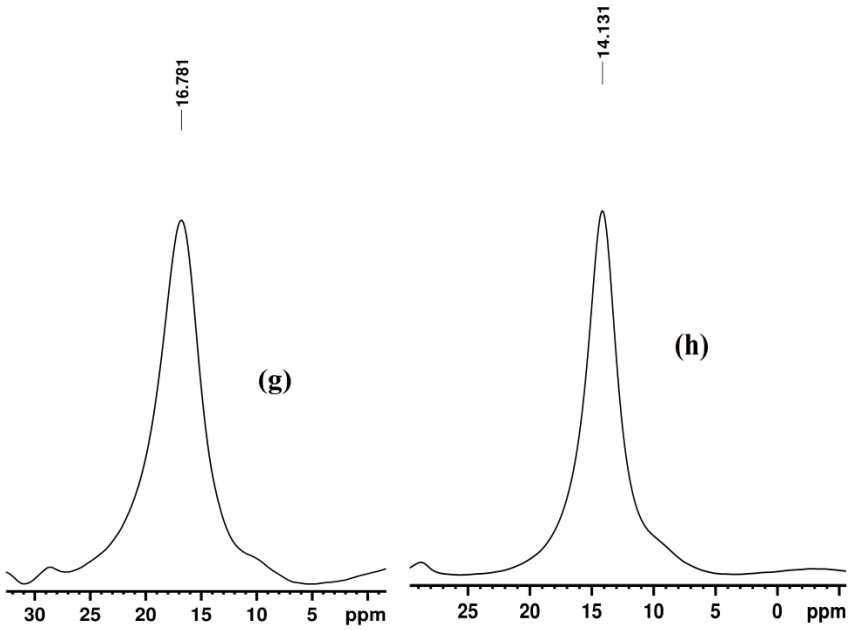


Fig.8S. ^{11}B NMR spectra of iminoboronate ester complex with (a) Mandelic acid (b) 2-Cl-mandelic acid (c) 4-Br--mandelic acid (d) 4-trifluoromethyl mandelic acid (e) 3,4-(Methylenedioxy)mandelic acid (f) 2-hydroxy-3-methyl butyric acid (g) Methyl-2,3-dihydroxy-3-phenyl propionate (h) Malic acid are acquired at 400 MHz NMR spectrometer.