Electronic Supplementary Material (ESI) for Dalton Transactions.

A Highly Stable Alanine Based Mono(aquated) Mn(II) Complex as T_1-weighted MRI Contrast Agent

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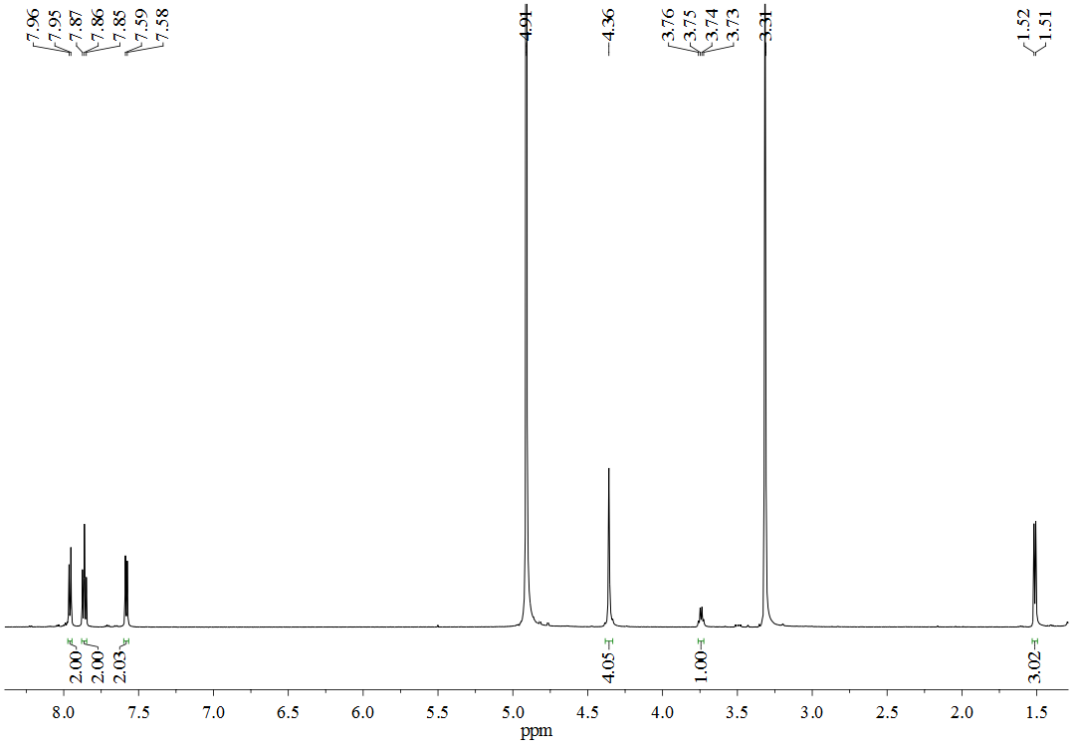

Figure S1. ^{1}H NMR spectrum for ligand Li_3cbda in CD_3OD solvent.

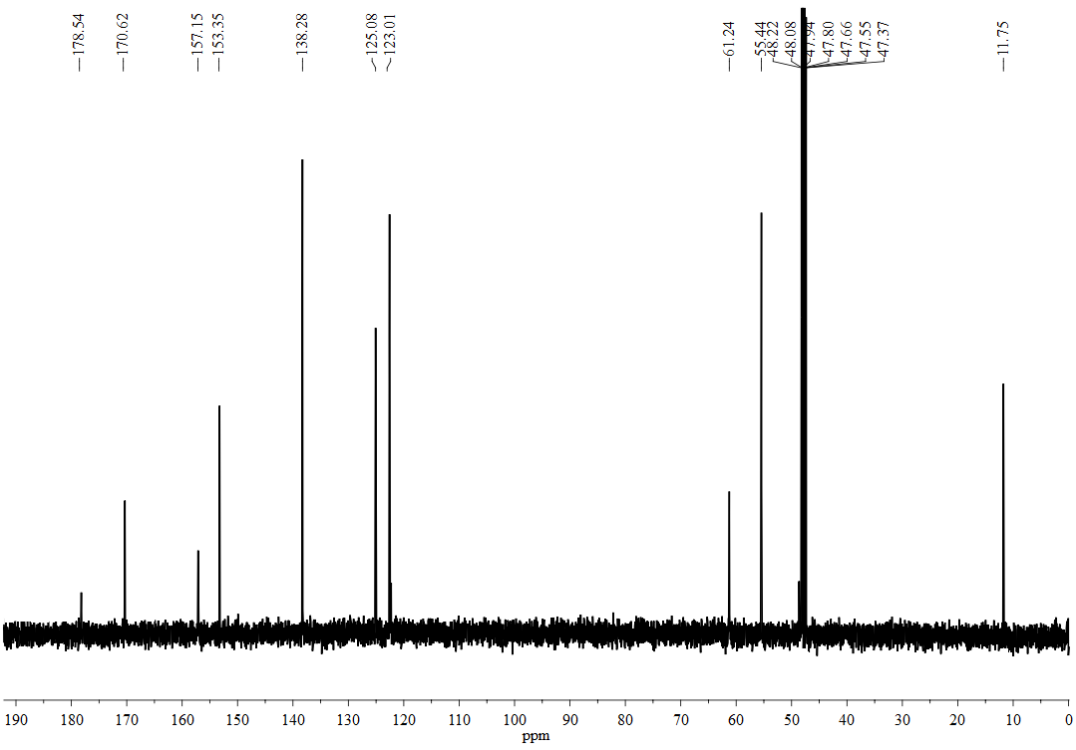

Figure S2. ^{13}C NMR spectrum for ligand Li_3cbda in CD_3OD solvent.

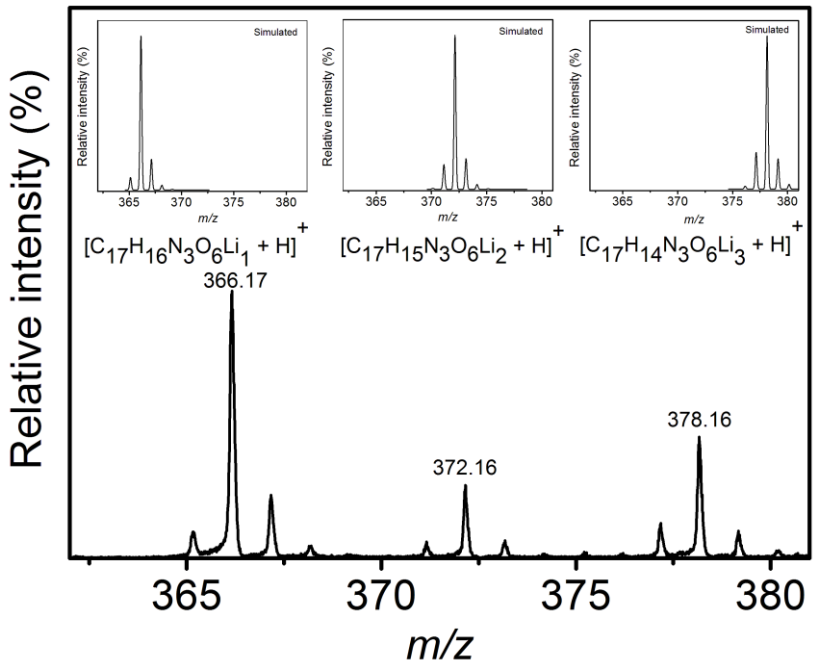

Figure S3. ESI-MS (+ve) mass spectrum of aquesous solution of ligand Li_3cbda. Simulated spectra have been been given as inset.

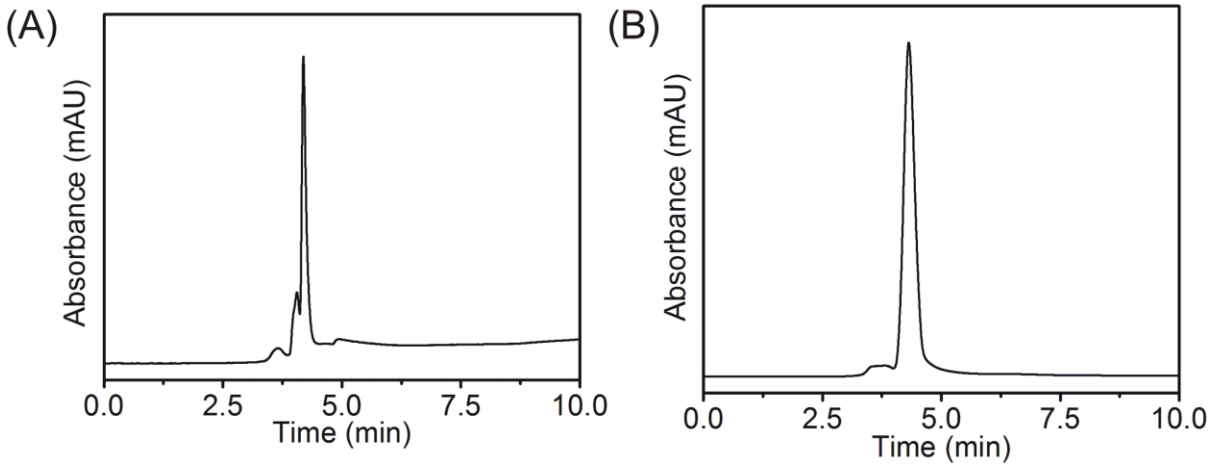

Figure S4. HPLC chromatograms of: (A) aqueous solution of the isolated ligand; (B) aqueous solution of the species obtained after 24 h stitrring of the ligand in the presence of 3 eqivalents of LiOH in water.

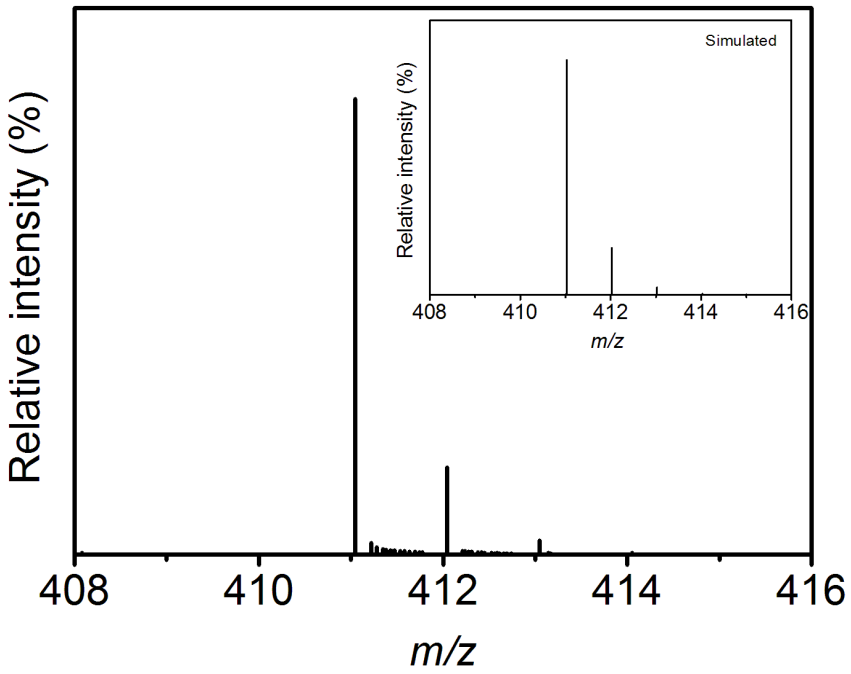

Figure S5. ESI-MS (–ve) mass spectrum of complex **1**. Simulated spectrum has been been given as inset.

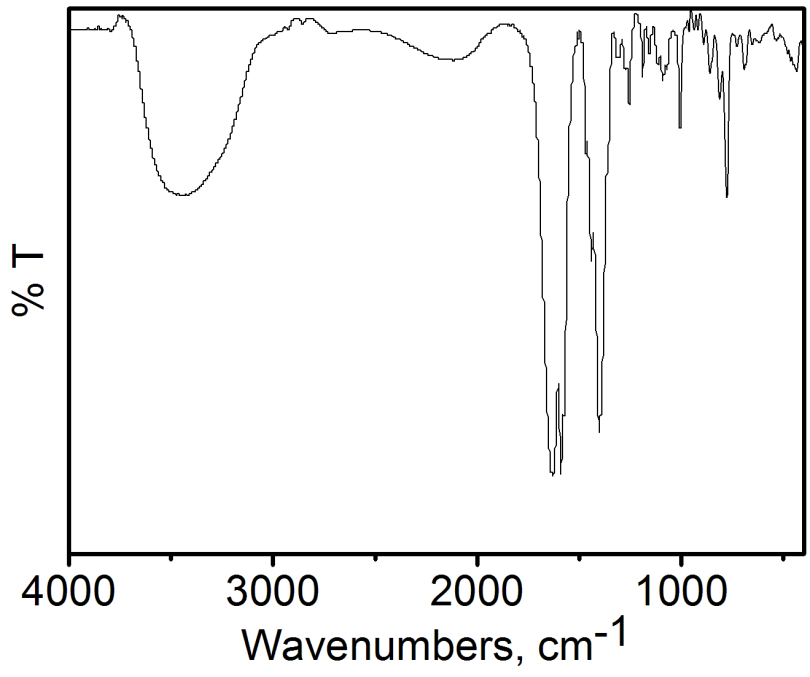

Figure S6. FTIR spectrum of ligand Li_3cbda.

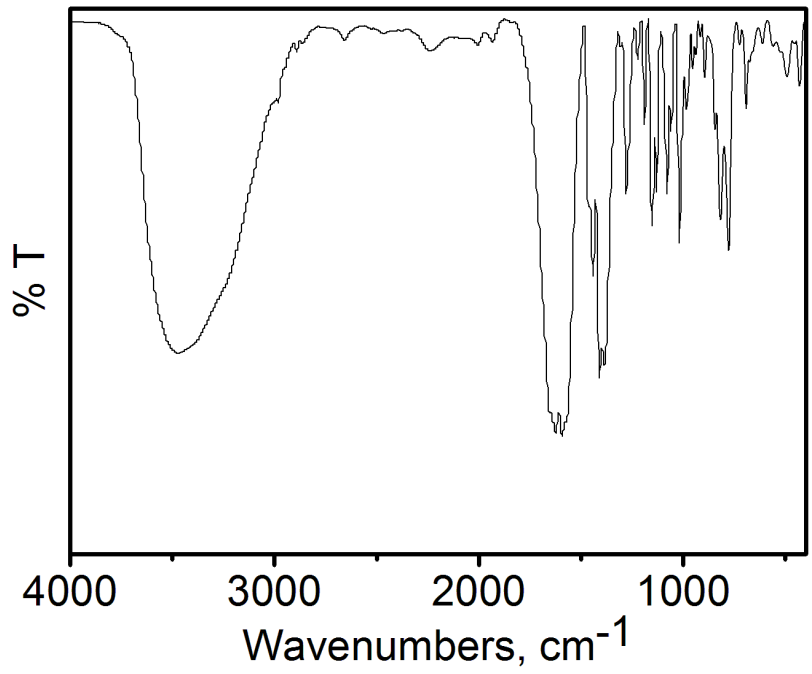

Figure S7. FTIR spectrum of complex **1**.

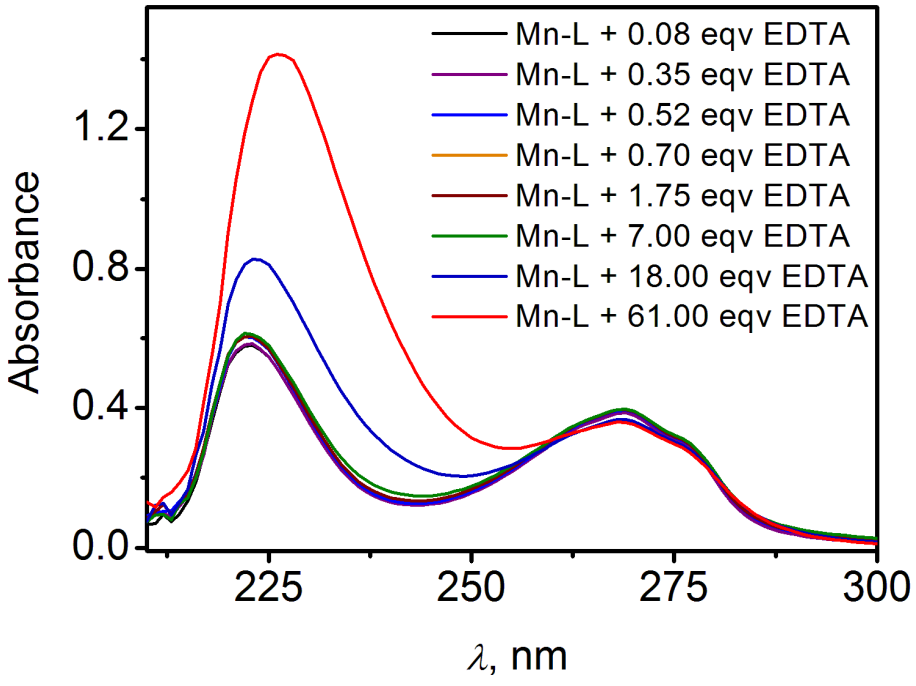

Figure S8. UV-Vis spectral changes during competitive study for determining pMn value for ligand Li_3cbda (where, L = Li_3cbda) against EDTA.

Competition titration with Na_2H_2EDTA:

The general procedure used to determine the pMn value for complex **1** was by competition titration method. Varying volumes of standardized EDTA stock solution were added to solutions containing constant concentration of ligand (Li_3cbda) and Mn(II) ion. The pH of all solutions was maintained at 7.4 by preparing all solutions in 10 mM HEPES buffer. All the solutions were kept for 24 hours to attain the thermodynamic equilibrium. The concentration of free and complexed ligand in each solution was determined from absorbance spectra considering a particular range of wavelength where spectral changes occurred. With respect to the absorbance of Li_3cbda, we determined the variation of absorbance values for each solution set which on further calculations gave the concentrations of Mncbda complex, MnEDTA complex, free Li_3cbda and free Na_2H_2EDTA for each set. Then we plotted the logarithim values of respective ratios for MnEDTA to Mncbda complex concentrations against logarithim of ratios for free Na_2H_2EDTA to free Li_3cbda concentrations for each set of samples. From the linear plot pMn value for the ligand Li_3cbda was calculated as its x-intercept value based on the equation given below.

$$\log([MnEDTA]/[Mncbda] = \Delta pM + \log(Na_2H_2EDTA]/[Li_3cbda]$$

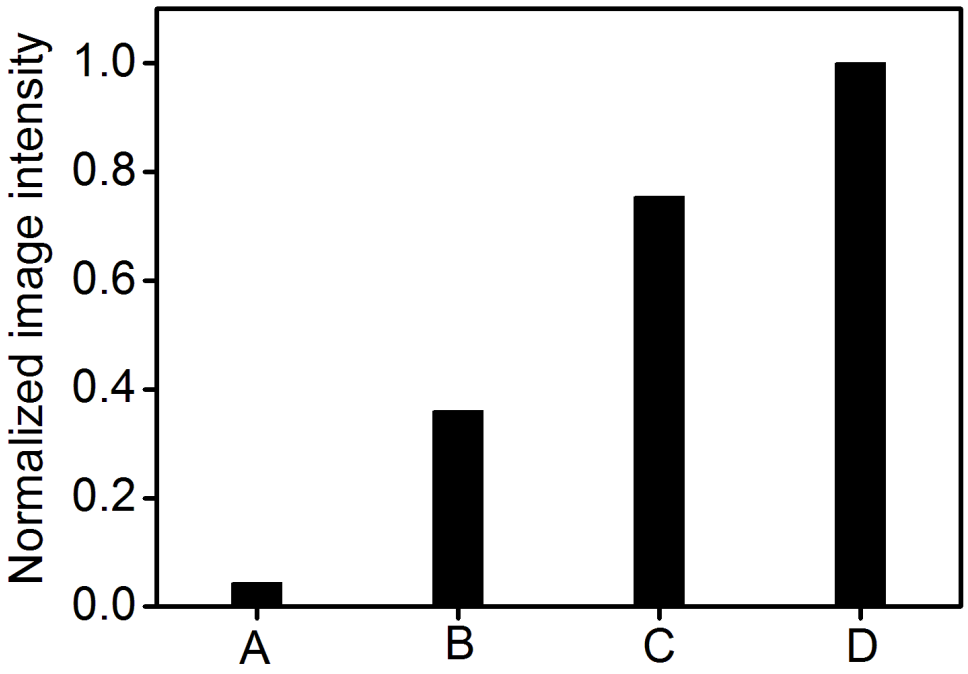

Figure S9. T_1-weighted image intensity plot for complex **1** at 1.5 T; where A = 0.25 mM, B = 0.50 mM, C = 0.70 mM, D = 1.00 mM concentrations of the aqueous solution of the complex at pH ~ 7.4 and 25 °C.