Supplementary Information for

An Analysis of the Conformational Behavior and Stability of the SAP and TSAP Isomers of Lanthanide(III) NB-DOTA-type Chelates

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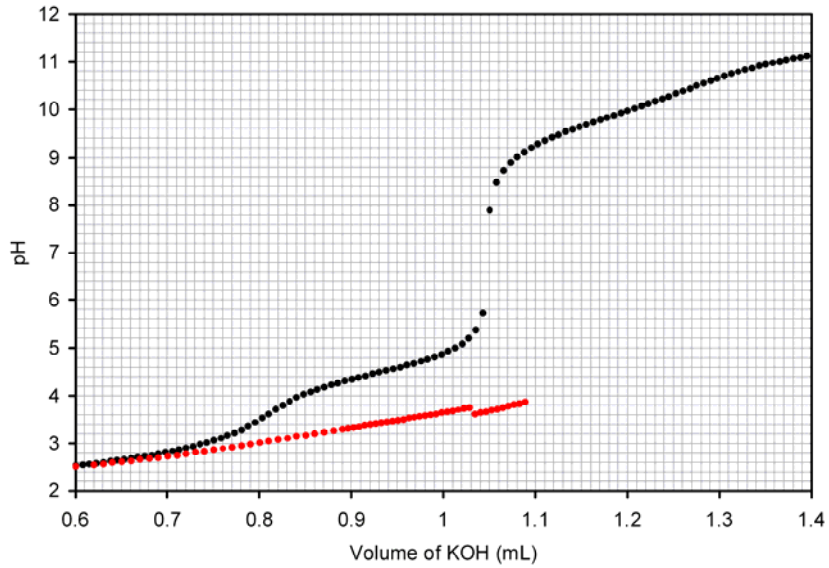

Figure S1. The titration curves of NB-DOTA in the absence and presence of Gd^{3+}, to determine the stability constant of the H_2GdL^+ intermediate.

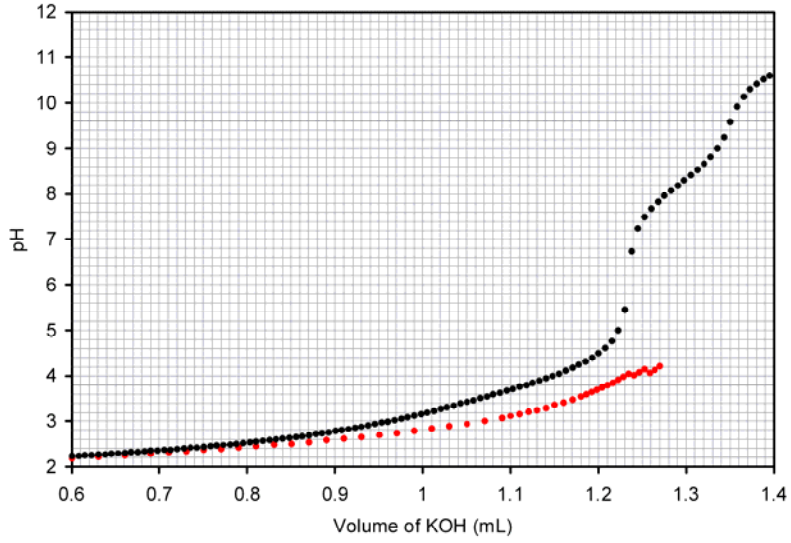

Figure S2. The titration curves of *S-RRRR*-NB-DOTMA in the absence and presence of Gd^{3+}, to determine the stability constant of the H_2GdL^+ intermediate.

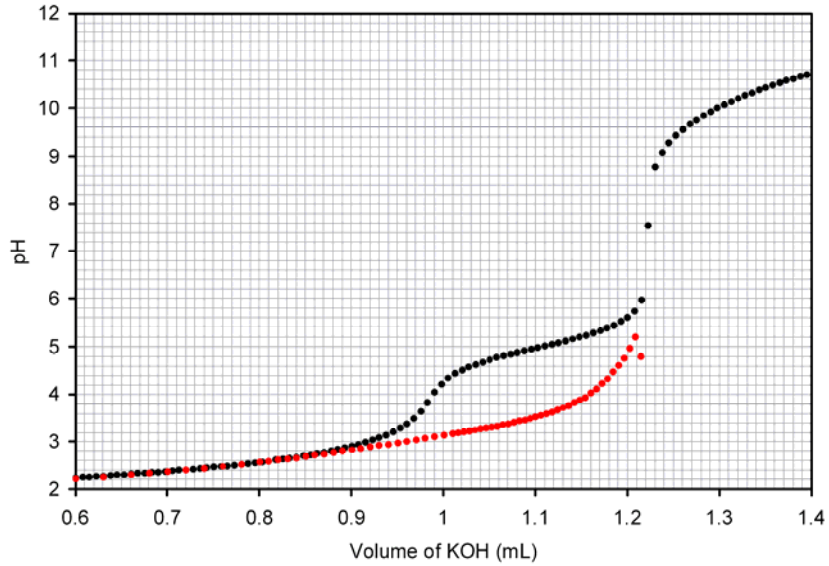

Figure S3. The titration curves of *S-SSS*-**1** in the absence and presence of Gd^{3+}, to determine the stability constant of the H_2GdL^+ intermediate.

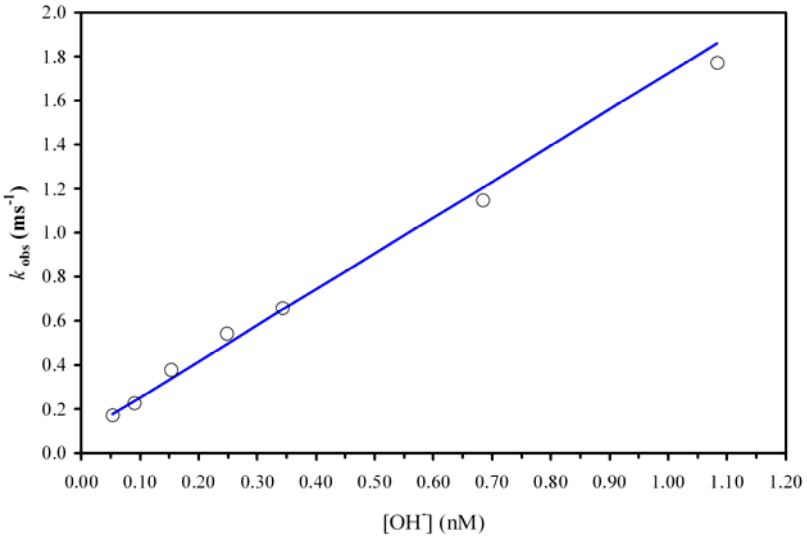

Figure S4. A plot of k_{obs} (the observation pseudo first order rate constant of chelate formation) against hydroxide concentration for GdNB-DOTA.

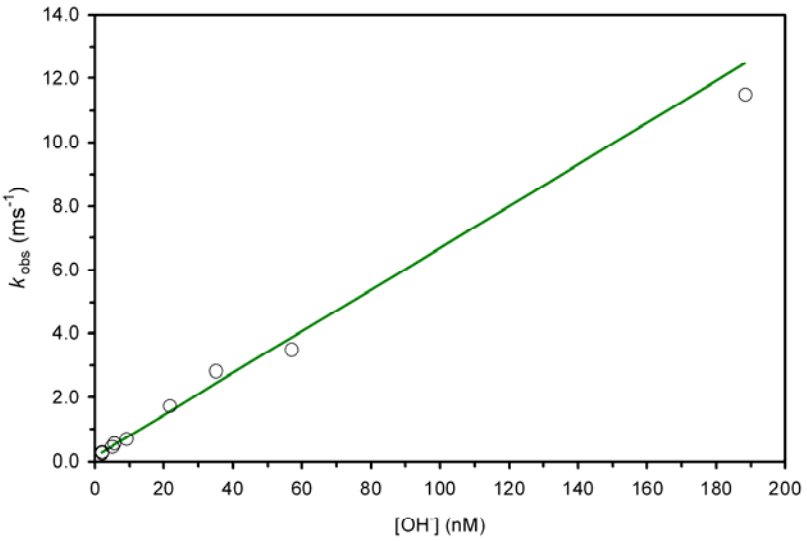

Figure S5. A plot of k_{obs} (the observation pseudo first order rate constant of chelate formation) against hydroxide concentration for Gd*S*-*RRRR*-NB-DOTMA.

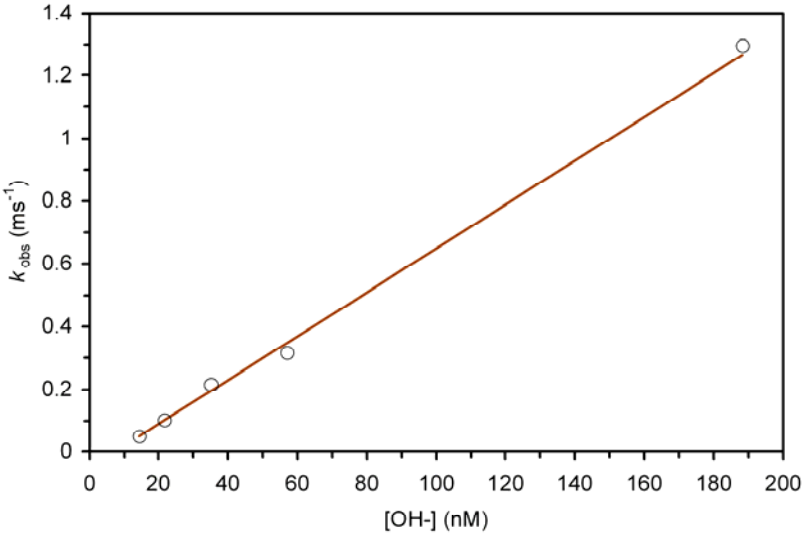

Figure S6. A plot of k_{obs} (the observation pseudo first order rate constant of chelate formation) against hydroxide concentration for Gd*S*-*SSS*-**1**.