

Supplementary Material for:

**Cerium, Europium and Ytterbium Complexes with Alcohol Donor
Groups as Chemical Exchange Saturation Transfer Agents for MRI**

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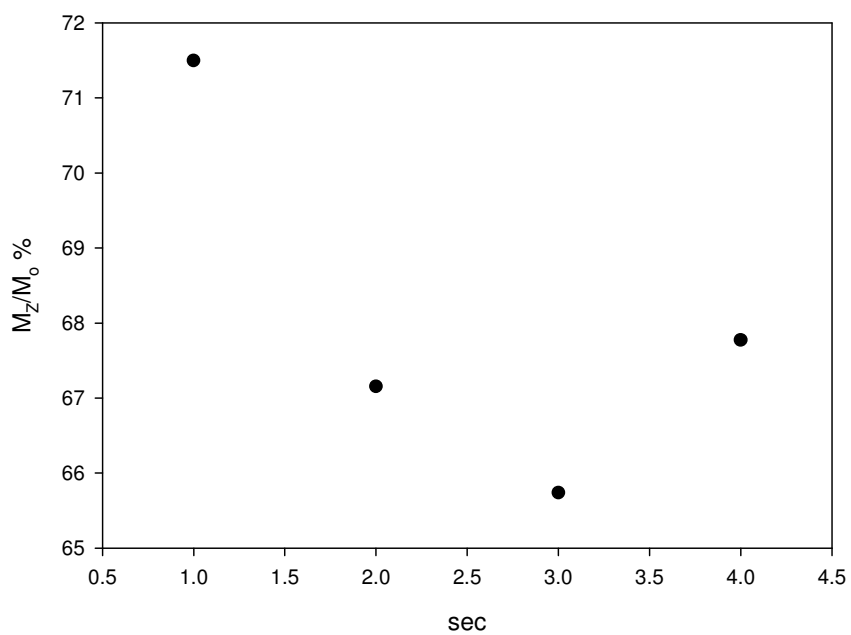


Figure S1. The CEST efficiency of the complex $\text{Ce}(\text{S-THP})^{3+}$ as a function of saturation time, $B_1=40$ db at room temperature, 20 mM MES buffer, pH 6.5, 100 mM NaCl.

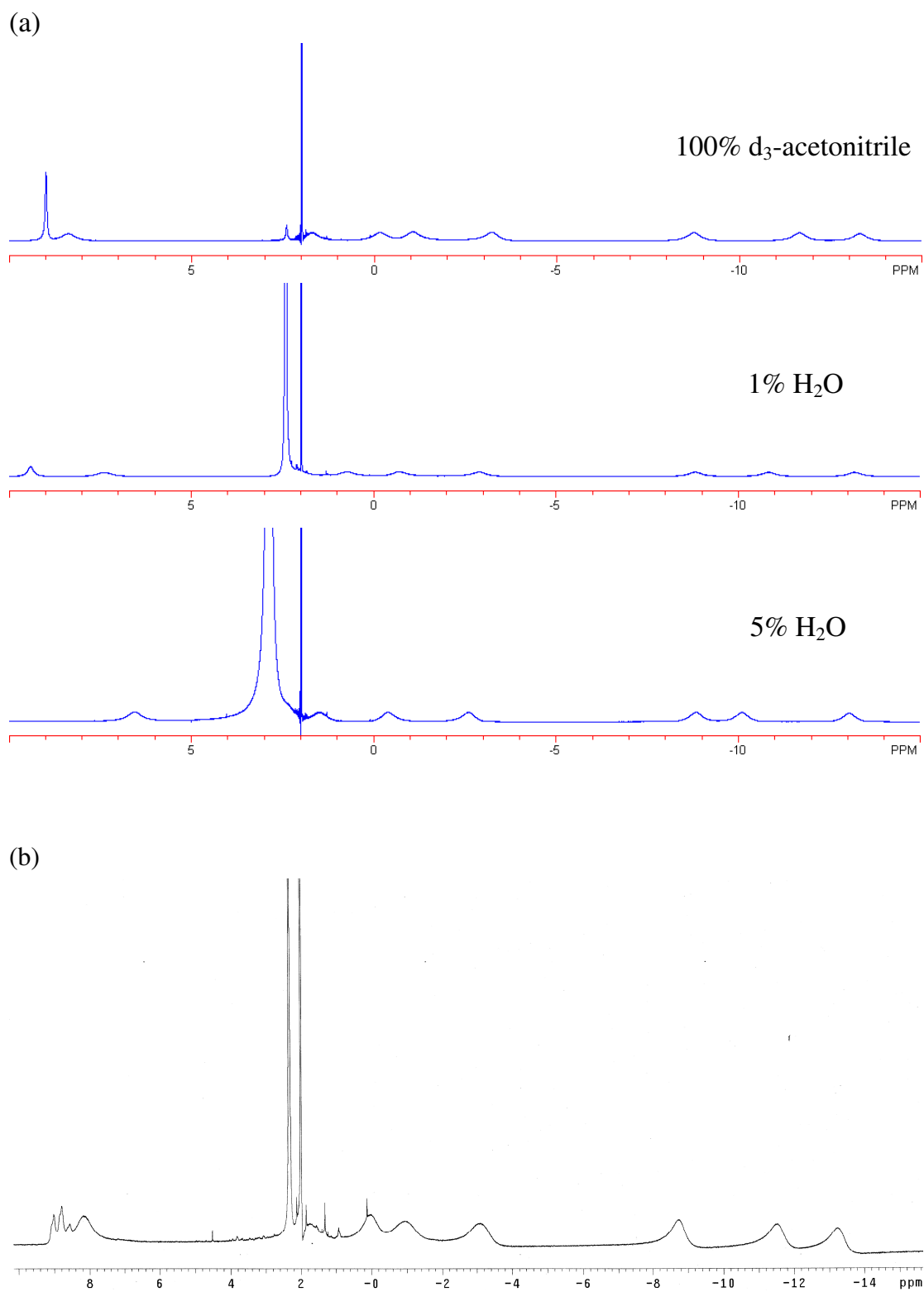


Figure S2. (a) ^1H NMR spectra of $\text{Eu}(\text{THED})^{3+}$ with different concentrations of water in d_3 -acetonitrile. (b) ^1H NMR spectrum of $\text{Eu}(\text{THED})^{3+}$ after partial H/D exchange.

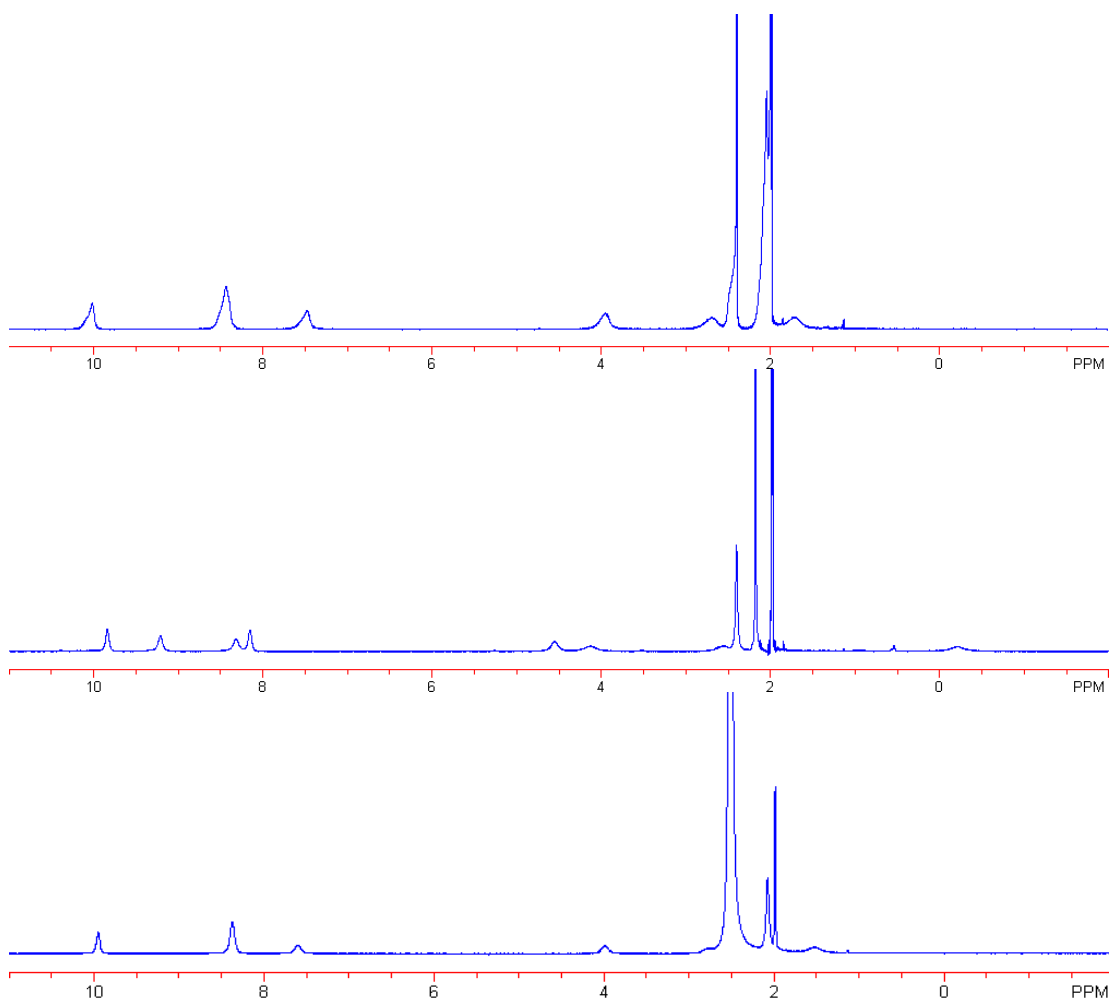


Figure S3. ¹H NMR spectra of Nd(S-THP)³⁺. Upper: sample in d₃-acetonitrile with addition of 1 drop of D₂O. Middle: sample in d₃-acetonitrile. Bottom: sample in d₃-acetonitrile with addition of 5 % H₂O.

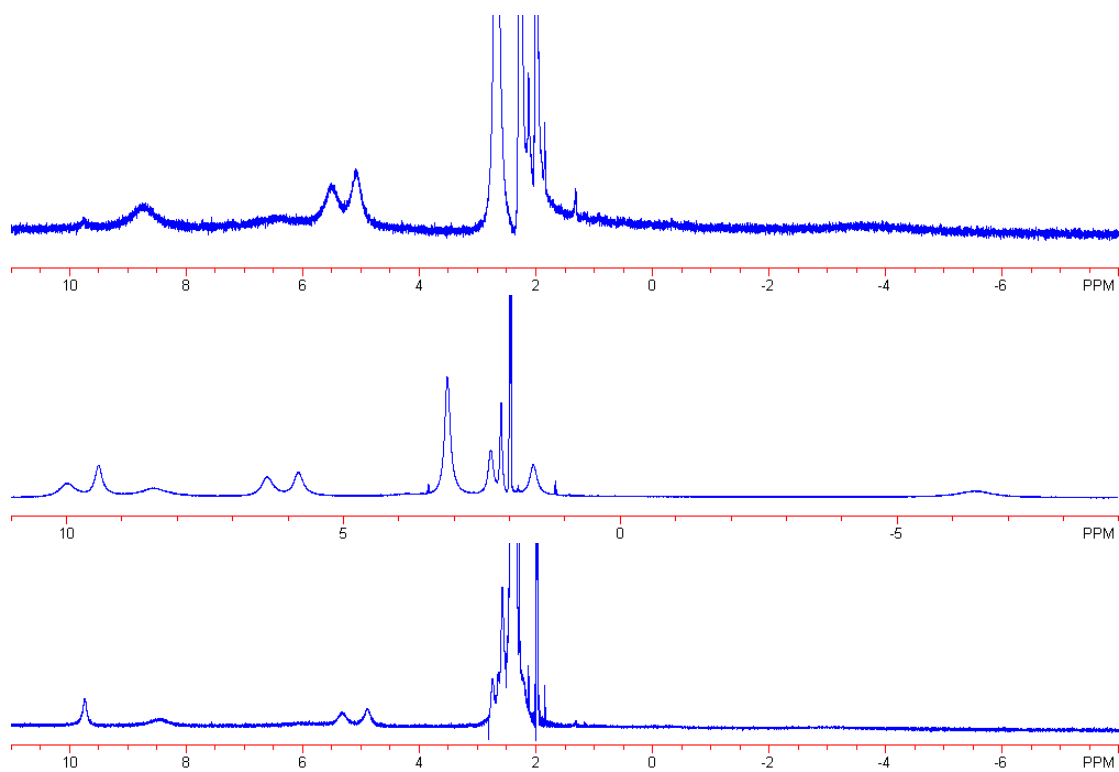


Figure S4. ¹H NMR spectra of Ce(S-THP)³⁺. Upper: sample in d₃-acetonitrile with addition of 1 drop of D₂O. Middle: sample in d₃-acetonitrile. Bottom: sample in d₃-acetonitrile with addition of 10 % H₂O.

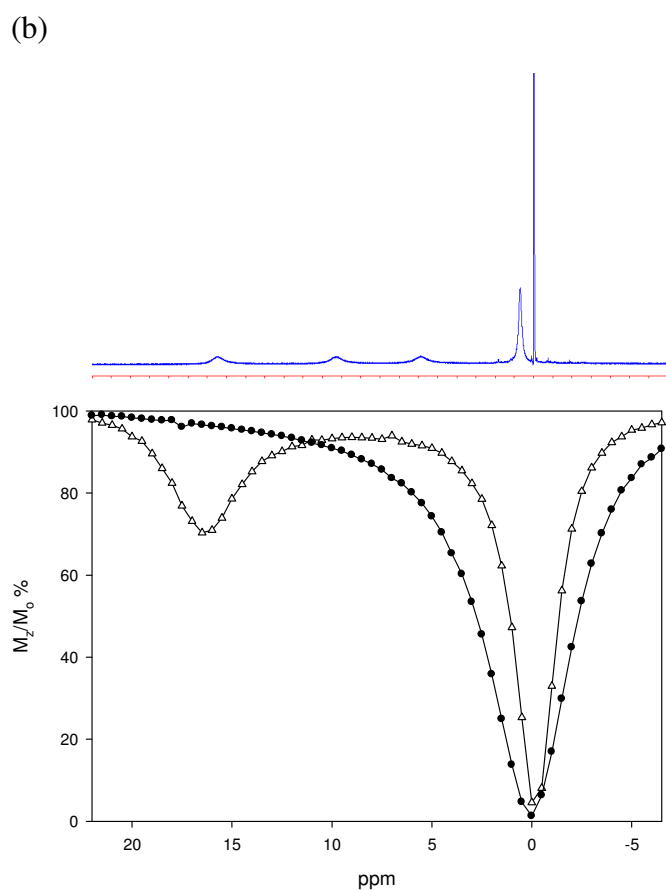
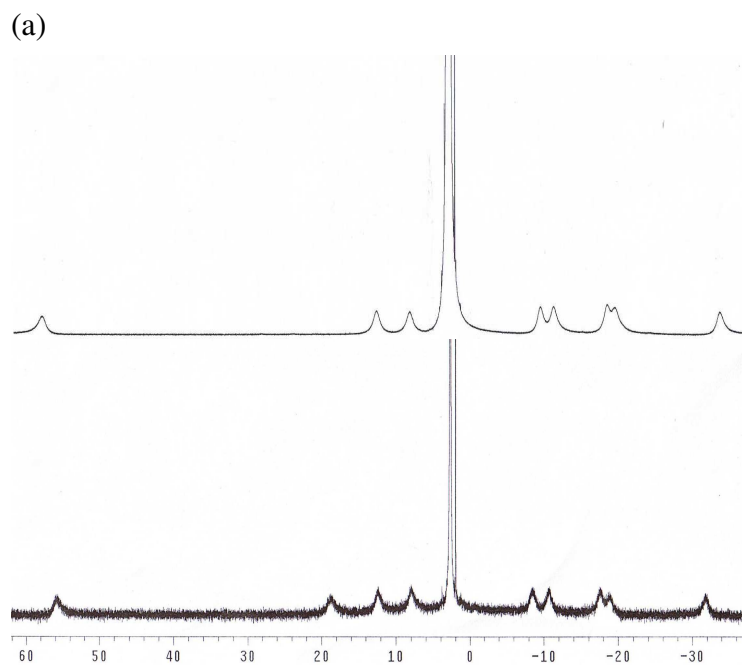


Figure S5. (a) $\text{Yb}(\text{THED})^{3+}$ dissolved in d_3 -acetonitrile (bottom) and upon addition of 1% H_2O (top). (b) CEST spectrum of 10 mM $\text{Yb}(\text{THED})^{3+}$ in d_3 -acetonitrile with no added water (Δ), addition of 1% H_2O (\bullet). The ^1H NMR spectrum shown on the top of the CEST spectrum is for the samples dissolved in dry d_3 -acetonitrile solution.

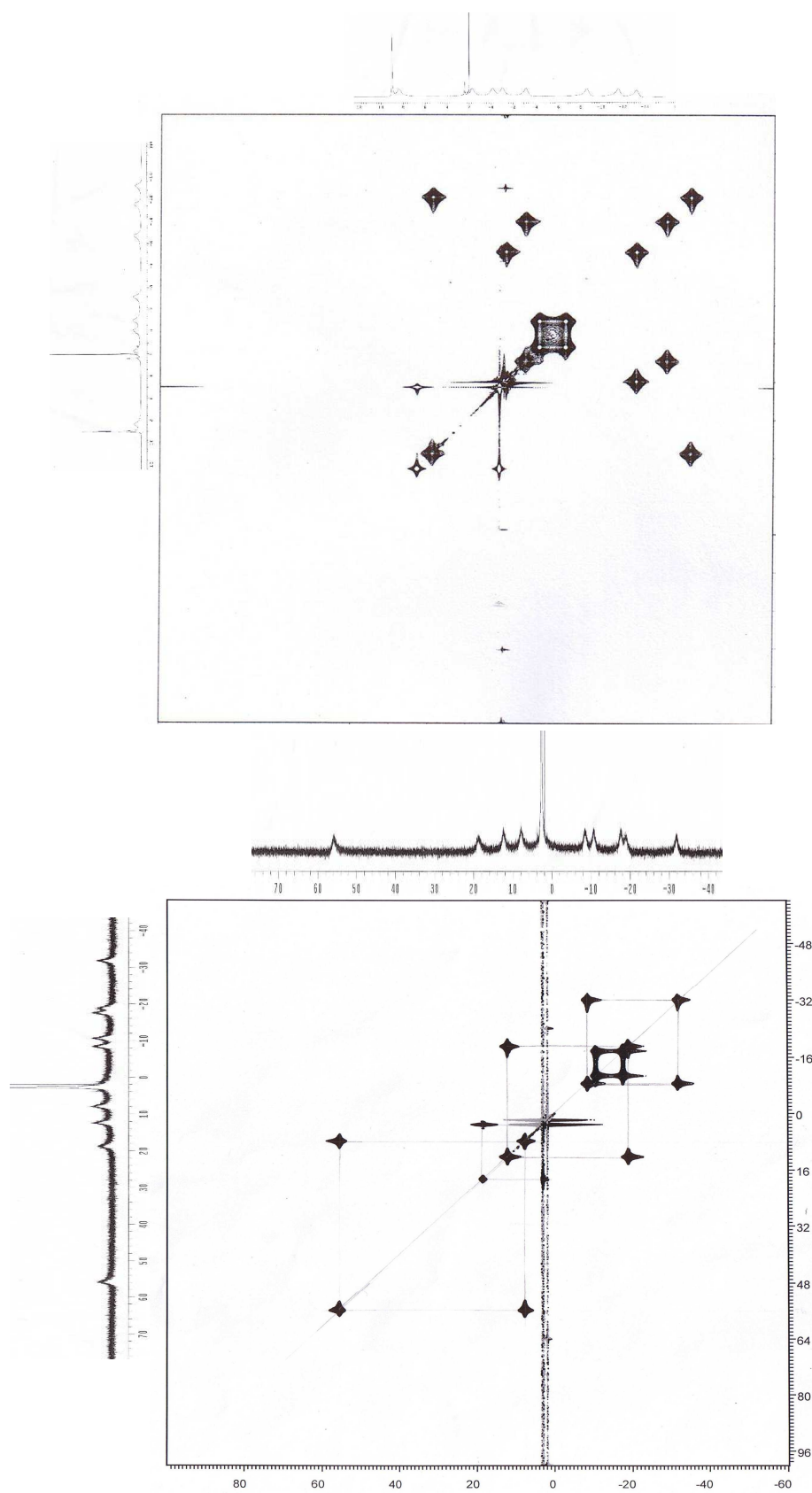


Figure S6. Two-dimensional exchange spectrum of $\text{Eu}(\text{THED})^{3+}$ (upper) and $\text{Yb}(\text{THED})^{3+}$ (lower) in d_3 -acetonitrile with 1% H_2O .

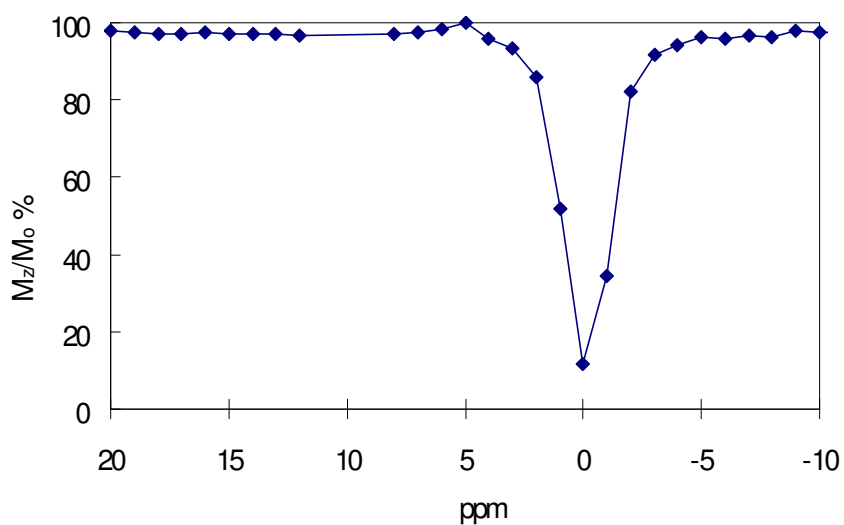


Figure S7. The CEST spectrum of 10 mM Nd(**S-THP**)³⁺ in d₃-acetonitrile with 5% H₂O.

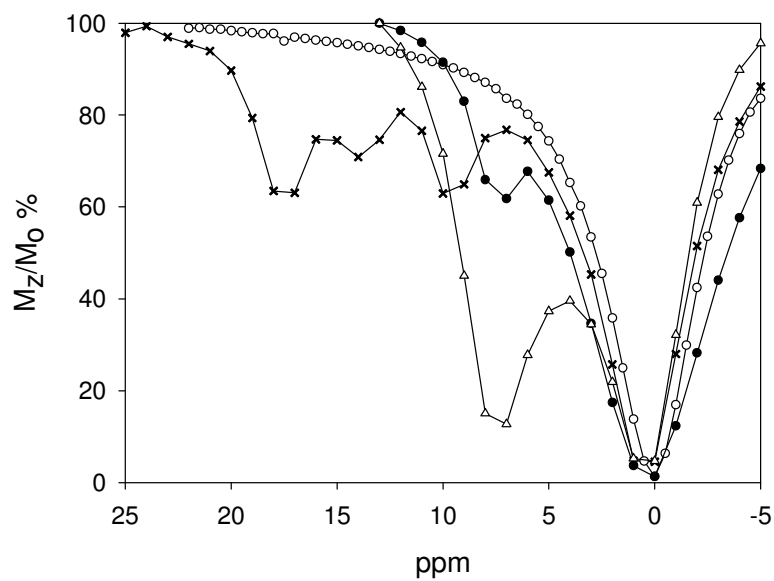


Figure S8. The CEST spectrum of 10 mM Ln(III) complex with addition of 1% H₂O in d₃-acetonitrile. ((Δ) Eu(**THED**)³⁺; (\circ) Yb(**THED**)³⁺; (\times) Eu(**CNPHC**)³⁺; (\bullet) Ce(**S-THP**)³⁺).

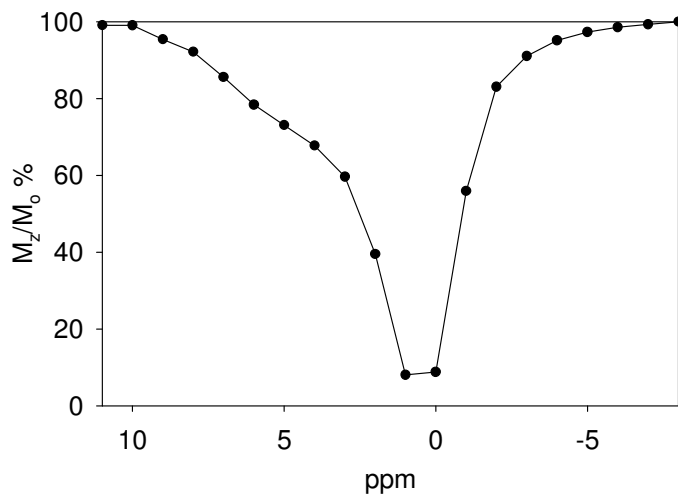
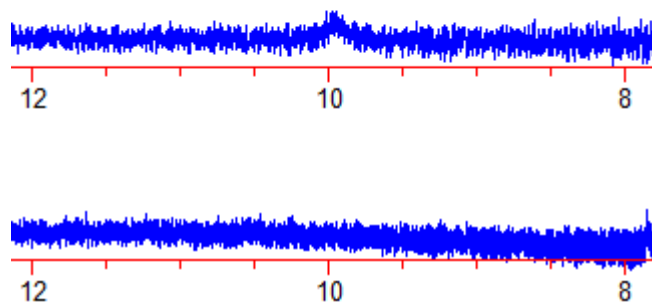


Figure S9. The CEST spectrum of 10 mM Eu(**THED**)³⁺ with 20 mM MES buffer, 100 mM NaCl at pH 5.6.

(a)



(b)

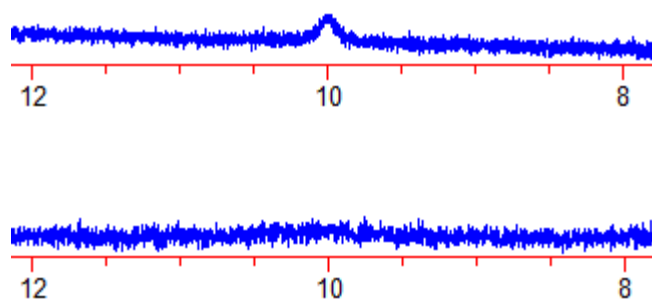


Figure S10. (a) 5 mM Eu(**S-THP**)³⁺ at pH 3.1 (upper) and pH 6.6 (lower). (b) 10 mM Ce(**S-THP**)³⁺ at pH 4.5 (upper) and pH 6.1 (lower).