Supporting Information to

Triethylenetetramine Penta- and Hexa-Acetamide Ligands and their Ytterbium Complexes as ParaCEST Contrast Agents for MRI

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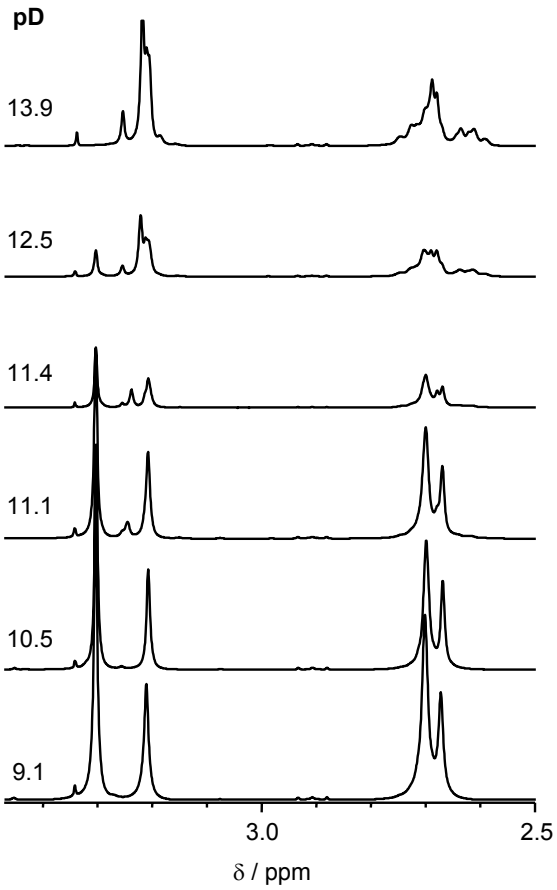

Figure S1. NMR spectra of ttham solutions (30 mM) in D_2O at various pD values between 9.1 and 13.9 (DNO_3, KOD, no buffer, 25°C). Chemical shifts (δ) are relative to the signal of sodium 3-(trimethylsilyl)-1-propanesulfonate (DSS, δ = 0 ppm) as the internal standard (c(DSS) = 3 mM).

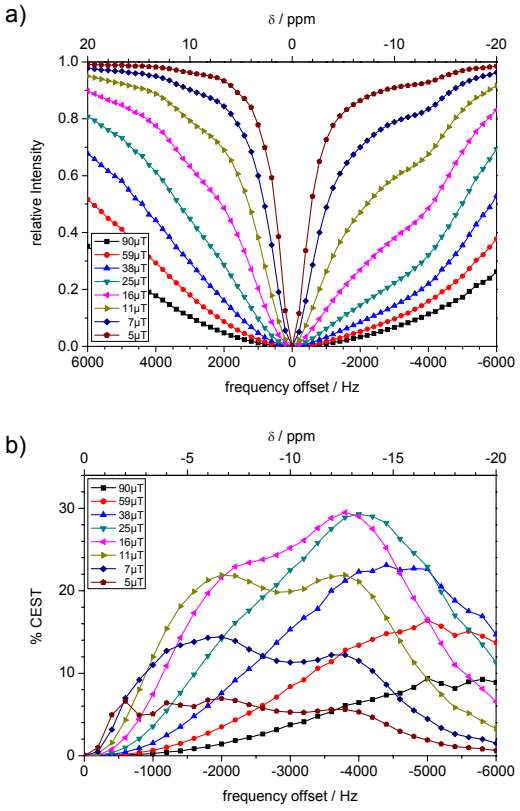

Figure S2. Proton Z spectra (a) and thereof calculated CEST spectra (b) of the Yb complex of ttaham in aqueous solution ($c(YbCl_3)$ = 20 mM, c(ttaham) = 22 mM, c(MOPS) = 10 mM, T = 310 K) at various presaturation power levels. Chemical shifts (δ) are relative to the resonance frequency of TMS (δ = 0 ppm), approximated by setting the solvent water protons at 4.75 ppm.

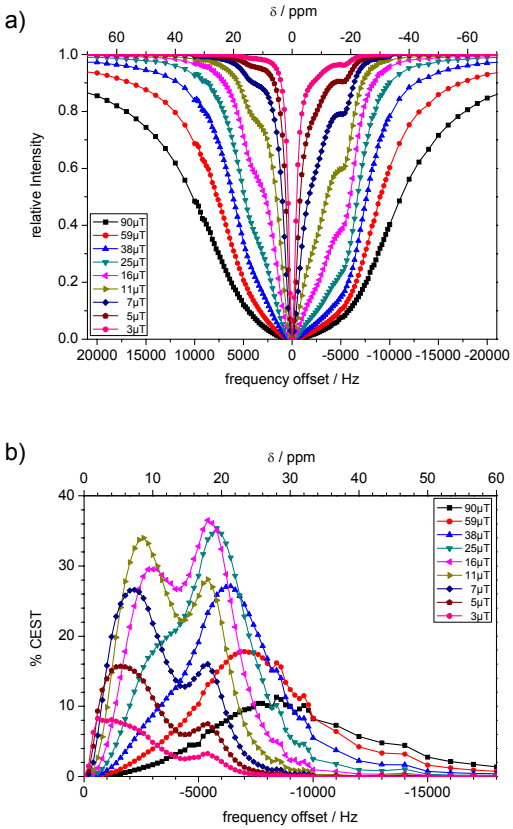

Figure S3. Proton Z spectra (a) and thereof calculated CEST spectra (b) of the Yb complex of dtpam in aqueous solution (c($YbCl_3$) = 20 mM, c(dtpam) = 22 mM, c(MOPS) = 10 mM, T = 310 K) at various presaturation power levels. Chemical shifts (δ) are relative to the resonance frequency of TMS (δ = 0 ppm), approximated by setting the solvent water protons at 4.75 ppm.