

Supporting Information to

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

Dirk Burdinski, Johan Lub, Jeroen A. Pikkemaat, Diana Moreno Jalón, Sophie Martial, Carolina*

Del Pozo Ochoa

Philips Research, High Tech Campus Eindhoven, 5656 AE Eindhoven, The Netherlands

AUTHOR EMAIL ADDRESS: dirk.burdinski@philips.com

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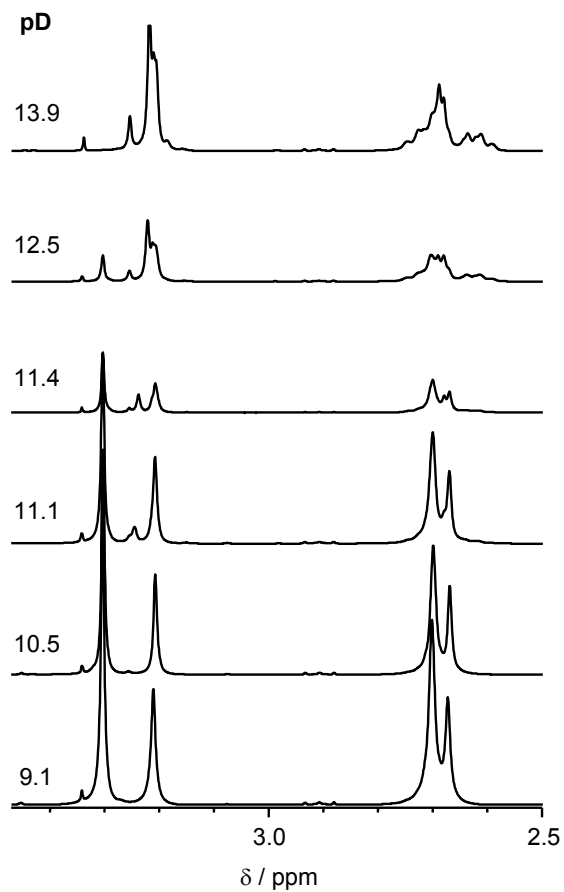


Figure S1. NMR spectra of ttham solutions (30 mM) in D₂O at various pD values between 9.1 and 13.9 (DNO₃, KOD, no buffer, 25°C). Chemical shifts (δ) are relative to the signal of sodium 3-(trimethylsilyl)-1-propanesulfonate (DSS, $\delta = 0$ ppm) as the internal standard ($c(\text{DSS}) = 3$ mM).

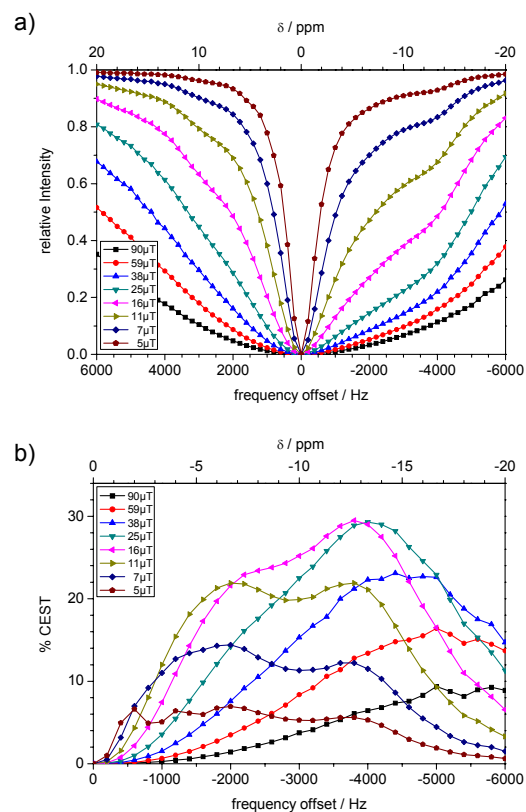


Figure S2. Proton Z spectra (a) and thereof calculated CEST spectra (b) of the Yb complex of ttaham in aqueous solution ($c(\text{YbCl}_3) = 20 \text{ mM}$, $c(\text{ttaham}) = 22 \text{ mM}$, $c(\text{MOOPS}) = 10 \text{ mM}$, $T = 310 \text{ K}$) at various presaturation power levels. Chemical shifts (δ) are relative to the resonance frequency of TMS ($\delta = 0 \text{ ppm}$), approximated by setting the solvent water protons at 4.75 ppm.

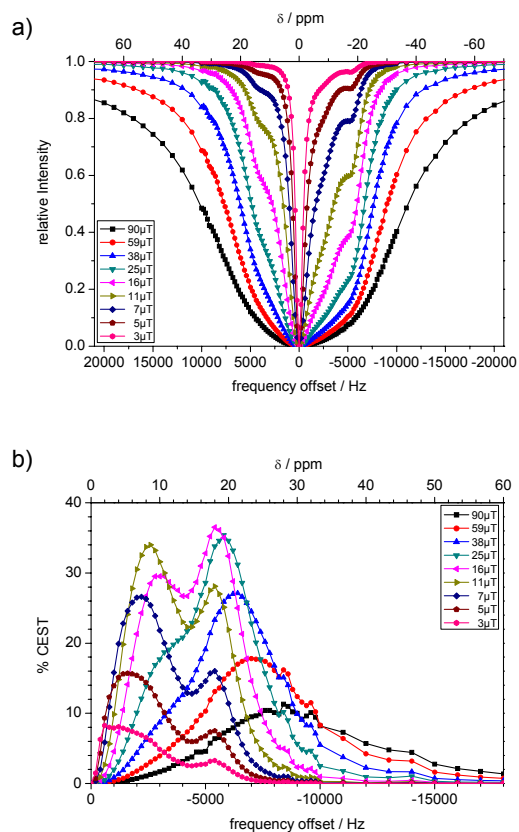


Figure S3. Proton Z spectra (a) and thereof calculated CEST spectra (b) of the Yb complex of dtpam in aqueous solution ($c(\text{YbCl}_3) = 20 \text{ mM}$, $c(\text{dtpam}) = 22 \text{ mM}$, $c(\text{MOPS}) = 10 \text{ mM}$, $T = 310 \text{ K}$) at various presaturation power levels. Chemical shifts (δ) are relative to the resonance frequency of TMS ($\delta = 0 \text{ ppm}$), approximated by setting the solvent water protons at 4.75 ppm.