

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Hyperpolarized  $^{89}\text{Y}$  NMR spectroscopic detection of yttrium ion and DOTA macrocyclic ligand complexation: pH dependence and Y-DOTA intermediates**<sup>1</sup> SARAH FERGUSON, ANDHIKA KISWANDHI, PETER NIEDEBALSKE, CHRISTOPHER PARISH, University of Texas at Dallas, ZOLTAN KOVACS, University of Texas Southwestern Medical Center, LLOYD LUMATA, University of Texas at Dallas — Dissolution dynamic nuclear polarization (DNP) is a rapidly emerging physics technique used to enhance the signal strength in nuclear magnetic resonance (NMR) and imaging (MRI) experiments for nuclear spins such as yttrium-89 by >10,000-fold. One of the most common and stable MRI contrast agents used in the clinic is Gd-DOTA. In this work, we have investigated the binding of the yttrium and DOTA ligand as a model for complexation of Gd ion and DOTA ligand. The macrocyclic ligand DOTA is special because its complexation with lanthanide ions such as  $\text{Gd}^{3+}$  or  $\text{Y}^{3+}$  is highly pH dependent. Using this physics technology, we have tracked the complexation kinetics of hyperpolarized Y-triflate and DOTA ligand in real-time and detected the Y-DOTA intermediates. Different kinds of buffers were used (lactate, acetate, citrate, oxalate) and the pseudo-first order complexation kinetic calculations will be discussed.

<sup>1</sup>The authors would like to acknowledge the support by US Dept of Defense award no. W81XWH-14-1-0048 and Robert A. Welch Foundation grant no. AT-1877.

Sarah Ferguson  
University of Texas at Dallas

Date submitted: 04 Nov 2015

Electronic form version 1.4