Abstract Submitted
for the 4CF09 Meeting of
The American Physical Society

Characterization of Manufactured Binding Sites in BPTI Using Laser Polarized ^{129}Xe[1] ZAYD MA, GEOFF SCHRANK, BRIAN SAAM, Department of Physics University of Utah, DAVID GOLDENBERG, Deparment of Biology University of Utah — We measure the NMR chemical shift of laser polarized ^{129}Xe in wild type, Y35G, Y23A, and F45S BPTI (Bovine Pancreatic Trypsin Inhibitor) solutions of varying concentration. Our technique uses ^{129}Xe in unprecedented low concentrations as a biosensor. The results provide structural information concerning the aforementioned proteins [2,3]. We use a flow-through polarizer that outputs ^{129}Xe hyperpolarized to $\sim$10%. Hyperpolarized gas coupled with a high resolution NMR spectrometer, enables us to measure sub-ppm chemical shifts at very low Xe and protein concentrations. In accordance with the fast exchange regime, we observe a single resonance that is chemically shifted as a function of protein concentration. Consistent with a rigid lattice and a manufactured binding site, Y23A and F45S demonstrate strong binding relative to wild type and Y35G. Wild type is believed not to have a specific binding site. Other experiments on Y35G have demonstrated a hydrophobic cavity and extensive solution-phase motion [1]. Weak binding supports the notion that a small fraction of solution-phase Y35G is in a conformation such that the cavity is accessible to Xe. [1] S. A. Beeser, *J. Mol. Biol.*, **269**, 154-164v [2] W. M. Hanson *et al.*, *J. Mol. Biol.* 2007, **366**, 230-243 [3] A. T. Danishefsky *et al.*, *Protein Sci.* 1993, **2**, 577-587

[1]Work Supported by NSF grant # PHY-0855482 and UURF.

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Date submitted: 22 Sep 2009 Electronic form version 1.4