Abstract Submitted
for the OSS14 Meeting of
The American Physical Society

Comparison of Amine Side-Chain Motion of Calbindin D-9k in Its Four Calcium Binding States by Molecular Dynamics Simulation MAHENDRA THAPA, Univ of Cincinnati — Calbindin D-9k, a small single domain, consists of a single pair of a helix-loop-helix motif (called EF-hand) that binds calcium with the ligands provided by the loop residues and helical residues immediately adjacent to the loop. It exits in four calcium binding states: a doubly loaded state (a state with a calcium atom in each of its two binding sites), two singly loaded states (a state with calcium in its first binding site only and a state with calcium in its second binding site) and an apo-state (a state with no calcium atom). Experiments have shown that calcium binding occurs in a positive cooperative fashion. This fact is also supported by computational studies on dynamics of backbone of the protein. Experimental Studies of the amine side chain dynamics of the doubly loaded state of the protein further enhances the point. To further investigate by computation, the molecular dynamics simulation approach has been used to study the amine side chain dynamics of all four calcium binding states of the protein. In the study, the different kinds of force fields, especially the AMBER (a molecular dynamics simulation suit) force fields, and different kinds of water models are employed in the GPU environment.

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Date submitted: 09 Mar 2014 Electronic form version 1.4