

ID: 10.1d

Title: Dynamic heterogeneity of temperature dependent dynamics of Cytochrome P450cam

Name: Yi, Zheng

Affiliation: ORNL/UT Center for Molecular Biophysics

The dynamic heterogeneity of temperature dependent dynamics of Cytochrome P450cam was studied by molecular dynamics simulation and elastic incoherent neutron scattering. It is shown that a q^4 correction to the elastic incoherent structure factor (where q is the scattering vector) can be simply used to reliably estimate from the experiment both the average mean-square atomic displacement (MSD) of the non-exchanged hydrogen atoms in the protein and its variance. The simulation results are in broad agreement with the experimentally-derived MSD and its variance derived from EINS on instruments at two different energy resolutions, corresponding to dynamics on the ~ 100 ps and ~ 1 ns timescales. MD simulation also confirms that the significant dynamical heterogeneity mainly arise from methyl-group rotations.