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Intrinsic Mean Square Displacement in Lysozyme DERYA VURAL, HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware, LIANG HONG, Oak Ridge National Laboratory — The internal dynamics of proteins is the essential interest of biophysics. The mean square displacement (MSD) of hydrogen in proteins and its associated hydration water is obtained by molecular dynamic (MD) simulation. The MSD as currently determined depends on the time of the MD simulation. A method is proposed in this paper to obtain the intrinsic MSD $\langle r^2 \rangle$ of hydrogen in the proteins. The intrinsic MSD is independent of the simulation time and defined as the infinite time value of calculated MSD that appears in the Debye-Waller factor. The method consists of fitting a model to the incoherent intermediate scattering function. The model contains the intrinsic MSD and a rate constant characterizing the motions of H in the protein. The method is illustrated by obtaining the intrinsic MSD $\langle r^2 \rangle$ of lysozyme in 100 ns and 1 μs MD simulations.

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