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A novel Generalized Langevin approach to bridge different timescales of relaxation in Protein Dynamics ESTHER CABALLERO MANRIQUE, Department of Chemistry, University of Oregon, JENELLE BRAY, Department of Chemistry, California Institute of Technology, MARINA GUENZA, Department of Chemistry, University of Oregon — The derivation of a Generalized Langevin Equation (GLE) for the long-time dynamics of biological systems presents several challenges as hydrogen bonding, secondary and tertiary structure, Coulombic interactions, and hydrophobic effects come into play. Here we propose a novel GLE approach where the internal friction is explicitly included in the protein dynamics, allowing the distinction between hydrophobic and hydrophilic effects. The protein is described as a linear chain of beads (centered at the alpha carbons) that are connected by harmonic springs. Input for our theory is short time (ns) molecular dynamics simulations of a single protein (or complex) in solution, in this case the bacterial signal transduction protein CheY. Effective inter-bead potentials and local friction coefficients are obtained from the simulations. A comparison of the bond autocorrelation function predicted from the theory and calculated directly from the simulation affords the test of the theory in the short timescales (ns). In the long timescales (ms), the theory is tested against experimental NMR T_1 relaxation values. Our results show a remarkable agreement in both cases, indicating that our GLE correctly bridges from the short- to the long-time scale of protein dynamics.

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