

THEORETICAL AND *IN SILICO* MODELING OF BIOLOGICAL SYSTEMS: FROM PROTEIN STRUCTURE PREDICTION TO CELLULAR DYNAMICS

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ABSTRACT

This thesis describes four distinct studies (involving a variety of concepts and methods from the physical sciences) of complex biological systems and processes that cover a wide range of time and length scales (extending from the molecular to the multi-cellular level), namely: 1) identification of near-native structures from a large set of *in silico* predicted structures for a given target protein by probing the stability of the structures against simulated heating using Molecular Dynamics (MD) simulations; 2) all atom MD simulation study of protein-cell membrane interactions designed to elucidate the relation between the conformational structure of the GP41 fusion peptide of HIV-1 virus and the density of the lipid membrane; 3) calculation of the potential of mean force for water transport through single wall carbon nanotubes from nonequilibrium MD simulations; and 4) development and application of a novel computational method, referred to as the cellular particle dynamics (CPD) method, for the simulation of the dynamics of multicellular systems.