Modeling protein-protein interaction with electrostatic polarization

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Abstract

Electrostatic interaction is perhaps the most important interaction in biomolecules, but so far the molecular force fields widely used to describe protein systems lack the polarization effect. Based on the recently developed fragment quantum method for proteins, we developed polarized protein-specific force field which takes into account polarization effect of specific protein structures. In this talk, we focus on the effect of polarization on interaction dynamics of protein-protein complex. Specifically, we studied the binding of Endonuclease colicins by a small immunity protein that binds with high affinity and specificity to protect against the cytotoxicity. The binding of Endonuclease colicin 9 (E9) by Immunity protein 9 (Im9) is found to involve some hotspots from helix III of Im9 on protein-protein interface that contribute the dominant binding energy to the complex. In the current work, MD simulations of the WT and three hotspot mutants (D51A, Y54A and Y55A of Im9) of the E9-Im9 complexes are carried out to investigate specific interaction mechanisms of these three hotspot residues using polarized protein force field.