Molecular modelling of site-specific DNA recognition by zinc finger protein assisted artificial metallonuclease

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Here we will present a molecular docking and dynamics study of the interaction between DNA and zinc finger protein linking with Ni(II) metallonuclease ligand. The ligand, in which the Ni^{2+} central cation chelates with a tripeptide, is able to cleave the nucleic acid effectively but the selectivity is not good. In order to make it selectively cleave DNA we bind it to the zinc finger protein sp1 in which the three fingers can recognize a DNA sequence with high specificity. The difficulty is that the crystal structure of sp1-DNA complex is not available. Therefore on the basis of the interaction between the base pairs and amino acid residues measured experimentally the protein is docked onto the DNA. The ligand is then connected to the protein through a flexible amino acid chain. Then the complex system is simulated in the explicit solvent through molecular dynamics. In this poster we will mainly focus on the molecular docking which is the fundamental step to build the model system. The basic principle, procedure, and the effectiveness will be discussed. We will also present the preliminary results of the molecular dynamics simulation.