Solvation effect on the protein docking process

: a molecular dynamics study

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Hydration water is believed to play an important role in the process of protein functional expression, for example in protein structural change, or in folding, or in the ligand binding process. The series of intense studies on the water hydration has been done through last several decades. It showed the characteristic chemical/physical parameters, that is, low diffusion constant[1], vectorial or anisotropic motion [2], and protein dynamics controlled by water motion [3]. These results suggest a strong correlation mechanisms between water and protein dynamics.

Recently, we have established a methodology to estimate the excess chemical potential or the solvation free energy in the use of trajectory data from MD simulation [4]. In the case of a single globular protein, the protein structural changes caused ~10^3kcal/mol solvation free energy change which strongly correlated with the density of the first hydration and the second hydration shell water.

In this study, under the motivation to investigate the solvation effect in the course of protein docking process, we calculate the solvation free energy of Barnase-barstar complex (PDBID:1BRS) [5]. From MD trajectory performed on each configuration, a solvation free energy was estimated by means of the classical MD simulation and the energy representation method [6]. We investigated the correlation between the solvation free energy depending on the distance and the configuration among two protein, the hydration water density, volume, and the solvent accessible surface area (SASA) of protein. These results suggest that the hydration water mediates the protei docking process. In the presentation, we will discuss on the global structural changes of Barnase-barstar complex on the framework of the solvation free energy.

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