

Theoretical Estimation of Difference in Hydrogen-Bond Free Energy of Biological Water and Bulk Water

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In this study, the difference in free energy to break hydrogen bond (H-bond) between bulk and biological water molecule was estimated by adopting a novel experimental approach. H-bond free energy between water molecules was measured using 7-azatryptophan (AW) as a probe molecule. The effect of hydrophilic surface toward H-bond free energy was compared through attaching AW onto the surface of a coiled-coil protein Alm. To validate experimental approach, we have performed molecular dynamics simulation. First, we have checked structural integrity of protein when AW is inserted. We have confirmed that protein maintains rigid α -helix coiled-coil structure while probe residues were stretched out toward opposite side of hydrophobic core of protein, well exposed to hydration environment. Second, we calculated H-bond free energy of bulk and biological water then compared with experiment value. Following Spoel's method, free energy of H-bond was related to lifetime of H-bonds. The H-bond free energy of the local biological water was higher than that of bulk water by ~ 0.3 kcal/mol, which agrees with experimental result.