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Thermodynamic properties of water solvating biomolecular surfaces

Matthias Heyden

Max-Planck-Institut für Kohlenforschung, Mülheim, Germany

Water molecules confined at ligand binding sites and biomolecular surfaces play an important role for binding affinities and kinetics. Restrictions of translational and rotational degrees of freedom of strongly bound or geometrically confined water molecules result in a decrease of molecular entropies. Releasing this water into the bulk upon ligand binding hence leads to an entropic gain, which can contribute significantly to the total free energy change. This simple picture of course doesn't contain any information on the potential energy change associated with the transfer of water molecules from the biomolecular surface into the bulk. Only both terms combined provide the local free energy of solvation, which competes with ligand binding processes. However, recent experiments are able to extract qualitative information on the local hydration water entropy via site-resolved measurements of water dynamics (1). This raises the relevant question, how much information on the local solvation free energy can be obtained from local hydration water entropy estimates. Here, we use explicit solvent molecular dynamics simulations to study thermodynamic and dynamic properties of water molecules hydrating biomolecular surfaces for a set of small proteins. We introduce a localized measure of the molecular entropy of hydrating water molecules based on the 2PT method for bulk liquids from Goddard and co-workers (2). This allows us to establish more quantitative correlations between dynamic and thermodynamic properties, in particular entropy, for water molecules in the vicinity of various biomolecular surfaces. Further, we can use our observations to determine how much we can learn about solvation free energies from local measures of hydration water entropy.

1. NV Nucci, MS Pometun, AJ Wand, Nat Struct Mol Biol 18:245-249 (2011).
2. ST Lin, M Blanco, & WA Goddard, J Chem Phys 119:11792-11805 (2003).

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Institut de Biologie Physico-Chimique
Laboratoire de Biochimie Théorique
13, rue Pierre et Marie Curie
75005 Paris

PSL RESEARCH UNIVERSITY