

Solvent-Induced effects on Protein Folding, Protein-Protein Association, and Molecular Recognition

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Abstract

Many biochemical processes such as protein folding or self assembly of proteins are highly specific. Proteins fold spontaneously into a very specific 3-dimensional structure. Proteins also associate spontaneously to form multi-subunit macromolecules. These processes occur in aqueous media. The question we pose is what is the role of water in these processes?

Until recently it was believed that the hydrophobic effect, i.e. the tendency of hydrophobic groups to “escape” from the aqueous environment is the dominant driving force for these processes.

Analysis of all the solvent induced contributions to the thermodynamic driving forces for protein folding and protein-protein association reveals that, contrary to the commonly accepted paradigm, hydrophilic interactions might be more important than hydrophobic interactions.

This conclusion was reached after critically examining the data on the various contributions to the driving forces for protein folding, and protein-protein association. Examples on the role of hydrophilic interactions on solubility of proteins, protein folding, protein-protein association and molecular recognition will be presented. Thus, hydrophilic interactions not only help in understanding the role of water in biochemical processes, but they can also be applied to design drugs that bind stronger to their targets.