Simulation of hydrogen bonds and solvation in ab initio calculation of protein folds

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Weak non-covalent interactions, such as coulomb, torsion and van der Waals forces determine shape and behaviour of molecules. Among these interactions, hydrogen bonds are certainly important. Evidences were gradually accumulated indicating that interactions energetically weaker than the ordinary OH /O bond of water and the NH / O bond of protein backbone, i.e. the CH / O, CH / N, OH / π and NH / π interactions, are also important. They are attractive electrostatic interactions of the type X-H···Y, in which Y, the hydrogen-bond acceptor, carries a full or partially negative charge, while the hydrogen-bond donor, X, is partially negative and H positive. To maximise the electrostatic attraction, the hydrogen preferentially approaches Y along the direction of one of its lone-pair orbitals.
We have developed two complementary approaches for the simulation of hydrophobicity and of hydrogen bond involved in protein folding.
The first one is namd internal and external solvation and describes the hydrophilic/hydrophobic intramolecular interactions and monitors the molecular water accessible surface.
The second one is hydrogen bond simulation by lone-pair orbitals taking into account the geometry of the H···Y interaction.
We will show the importance of these two procedures in protein folding simulation.