STRUCTURES AND ENERGETIC OF THE H-BOND NETWORKS IN AQUEOUS SOLUTION OF ALANINE

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ABSTRACT: Structures and energetic of the hydrogen bond (H-bond) networks in aqueous solutions of alanine (Ala) were investigated using various computational techniques. The test-particle model (T-model) was applied in the calculations of the intermolecular potential between Ala and water. Various conformations of Ala were considered in Molecular Dynamics (MD) simulations and hydration free energy calculations. In the present work, the Thermodynamic Integration (TI) method was proven to be the most suitable approach for the hydration free energy calculations. The behavior of water molecules in the H-bond networks at the functional groups of Ala was analyzed and discussed based on Probability Distribution (PD) maps and potential energy landscapes. The preferential conformation of Ala in aqueous solution inferred from the hydration free energy profile is to be ϕ = 180 and ψ = 200 degree.

KEYWORDS: H-bond, alanine, T-model, molecular dynamics simulations, hydration free energy