FREE ENERGY OF HYDRATION FOR ALANINE ZWITTERION

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ABSTRACT: Molecular Dynamics (MD) simulations in combination with Thermodynamic Integration (TI) method were applied in the calculations of hydration structures and energetic of alanine zwitterion (Alaz) in aqueous solutions ($[Alaz]_{aq}$). The investigations started with construction of the Test-particle model (T-model) potential to describe the interaction between water and Alaz, followed by MD simulations of $[Alaz]_{aq}$ at 298 K. The MD results suggested the hydration free energy profiles as well as the shapes of the potential energy landscapes of the hydrogen bond (H-bond) networks at the charged functional groups of Alaz. The information on the three-dimensional structures and the dynamic behavior of water molecules in the vicinities of the functional groups of Alaz in aqueous solutions was discussed in detail.

KEYWORDS: alanine zwitterion, free energy, thermodynamic integration