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Theoretical Investigation of Structures, Thermodynamics and Reactivity of Dipeptide Molecules Based on Multidimensional Free Energy Maps

(Rutgers University)○Tateki Ishida・Ronald M. Levy

The structure, thermodynamics and reactivity of conformational changes of a series of dipeptides protein is investigated based on multidimensional free energy (potential of mean force) profiles. The free energy surfaces are generated by using umbrella sampling and the weighted histogram analysis method. The analytical generalized Born model including nonpolar hydration is employed to take solvent effects into account.

Two representative torsion angles (for example, phi and psi for alanine dipeptide) are selected as reaction coordinates and two-dimensional free energy surfaces are estimated. As an exmaple, we find that the free energy profile of alanine dipeptide is in very good accord with high resolution experimental data extracted from the PDB (Protein Data Bank) of phi and psi dihedral angle distributions observed for alanine residues in proteins. Also, we estimate the existence probability around a minimum point for each conformation, and discuss its dependence on temperature considering the possibility to observe a conformation with small lifetime experimentally in single molecule experiments. On proline dipeptide, we observe that the results of the relative free energy between minima and the free energy surface profile depend on the selection of reaction coordinates. Based on this fact, the way of choosing reaction coordinates for a variety of amino acid types will be discussed. We will also discuss the dynamics of conformational change.