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Molecular Dynamics Simulated Annealing Study of Gramicidin A in Water and the Hydrophobic Environment TAKAHARU MORI, YUKO OKAMOTO, Department of Physics, School of Science, Nagoya University and JST-BIRD — Gramicidin A is a hydrophobic 15-residue peptide with alternating D- and L-amino acids, and it forms various conformations depending on its environment. For example, gramicidin A adopts a random coil or helical conformations, such as $\beta^{4.4}$-helix, $\beta^{6.3}$-helix, and double-stranded helix in organic solvents. To investigate the structural and dynamical properties of gramicidin A in water and the hydrophobic environment, we performed molecular dynamics simulated annealing simulations with implicit solvent based on a generalized Born model. From the simulations, it was found that gramicidin A has a strong tendency to form a random-coil structure in water, while in the hydrophobic environment it becomes compact and can fold into right- and left-handed conformations of β-helix structures. We discuss the folding mechanism of the β-helix conformation of gramicidin A.

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