

Free-energy landscape of peptides in explicit water obtained from molecular dynamics simulation

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The conformational space of a peptide/protein is multi-dimensional and the potential energy (i.e., conformational energy) surface generally involves a number of energy local minima. This complexity in the energy surface has been causing a difficulty in the conformational sampling of peptide/protein computationally done. To effectively sample the space, we have developed an enhanced conformational sampling method, multicanonical molecular dynamics simulation, and applied it on peptide systems in explicit water. The free-energy landscape, obtained from the sampling, provided thermodynamically stable conformations at a room temperature and pathways for the conformational changes among the stable conformations. The stable conformations correlated with experimentally determined structures. In the landscape, semi-stable conformational clusters consisting of secondary-structure elements were also found. The property of the landscape may propose a key to understand protein folding.