Simulations of Peptide Folding

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Abstract

Introduction:

Together with the increasing of small peptide design for medicinal and industrial applications, peptide simulations become more important and this leads to the development of peptide simulation methods. Thus, we can study peptide folding dynamics with details by the different methods of simulations. In addition, can be described the kinetics and thermodynamics of peptide forming. However, existing methods in terms of constraints and cost calculations are diverse and should be chosen carefully.

Methods: Molecular Dynamics (MD) simulations as a physics-based method is used widely in biomolecular studies. Replica-Exchange MD (REMD) is a special protocol of MD that simulate peptide folding well. In this method, several MDs perform at different temperatures on the peptides. In addition, there are many software that use ab-initio calculations for the structure prediction of the peptide. PEP-FOLD3 is the newest and most efficient of them that can predict the structure of peptide to 50 amino acids.

Results and discussion: Many fragments of peptide simulated by REMD under the different conditions, such as variant force-fields and water models and the results compared with the natural properties of peptides. These studies show good agreements.

Conclusion: the peptide folding methods and their different conditions are studied well and according to, we can use the optimum conditions and methods to study new peptide, based on expected goals.

Keywords: Replica Exchange Molecular Dynamics, REMD, PEP-FOLD3

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