MOLECULAR DYNAMICS SIMULATION PROTEIN L IN WATER AND UREA 8 M

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INTRODUCTION

Protein folding mechanism is an important aspect in biochemistry that related with biological activity. The protein folding mechanism provides information about how the native structure of the protein was formed and also how the most stable structure of the protein. In this research we have performed unfolding simulation of domain B1 of Protein L. Folding mechanism could be obtained from unfolding simulation.

MATERIALS AND METHODS

These Simulations were performed in explicit solvent making use of the Amber 9 Molecular Dynamics (MD) package. The initial structure for Protein L was obtained from Protein Data Bank (PDB) entry 1HZ6 (Jason *et al*. 2001). We used 8 Å reaction field cutoff. The water model used TIP3P and urea concentration is 8 M.

The system was prepared to energy minimization and equilibration, and then gradually heated to 400 K and 500 K as constant temperature. Higher temperature is more efficient for unfolding simulations because it leads to faster unfolding (Hongxing *et al*. 2008) Finally, the MD simulations were carried out and the trajectory of the protein were saved every 2 fs for structural analysis.

RESULTS AND DISCUSSION

The unfolding simulation of protein L was simulated in water and 8 M urea solutions. The first simulation was performed at 500 K. The protein in water has been observed to unfold in 4,8 ns in an MD simulation and in 8 M urea solution unfold in 4,2 ns (see Fig 1).

The second simulation was performed at 400 K. Only the protein in urea has been observed to unfold in 18 ns in an MD simulation (see Fig 2). During 30 ns MD simulation the structure protein

in water was relative stable, the rms deviation (RMSD) fluctuated at 4 Å. That simulation describe, the unfolding process caused denaturant agent 8 M urea solution.

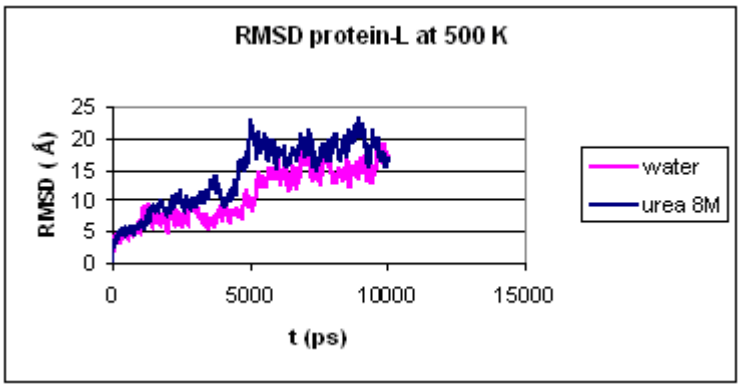

Fig 1. Root Mean Square Deviation unfolding simulation protein L at 500 K

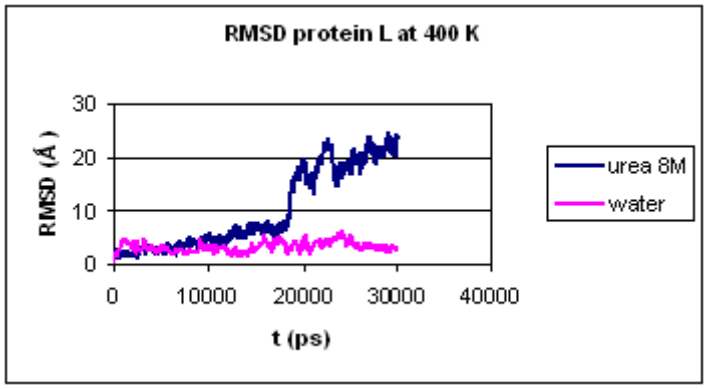

Fig 2. Root Mean Square Deviation unfolding simulation protein L at 400 K

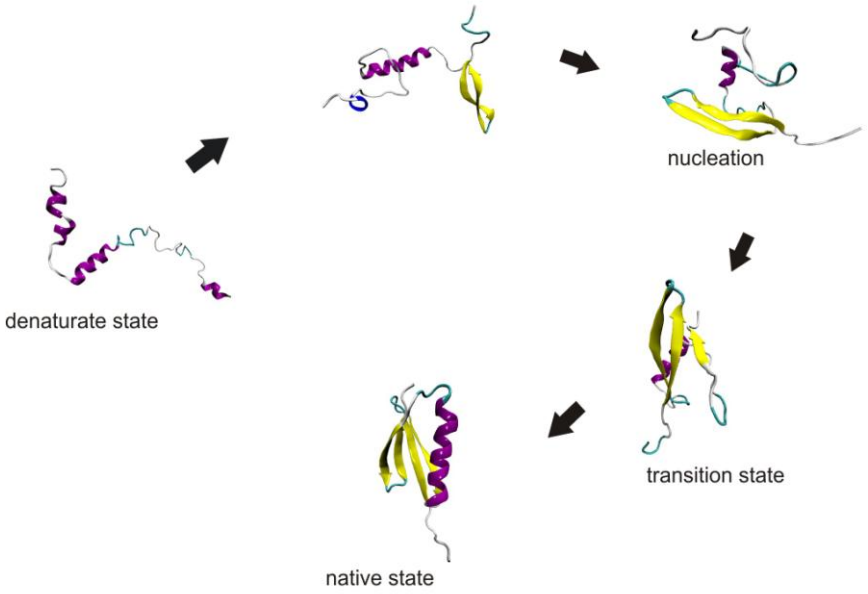

Fig 3. Folding mechanism of protein L

In figure 2, the RMSD protein L in urea 8 M was increase drastically at 18 ns time simulation. It can related the unfolding of protein L following a two-state transitions, from native structure direct to denatured state without intermediate state (Scalley, et al. 1997) Further inspection to the simulation trajectory suggested that folding mechanism of protein L following the model of nucleation condensation (see Fig 3)

REFERENCES

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