

Thermophilic proteins – exploring thermal stability of FN3 domain from *Thermoanaerobacter tengcongensis* based on *in silico* experiments

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Streszczenie

Extremophilic proteins exhibit a remarkable stability under extreme conditions (e.g. thermophilic systems are stable at elevated temperatures), offering insights into molecular adaptations and early life on Earth. Currently, thermophilic organisms are widely investigated, and they constitute a challenge for new industrial and pharmaceutical applications. Examples of studies on extremophiles, including thermophiles, reach as far as space exploration experiments. The Fibronectin Type 3 (FN3) domain, a conserved structural motif, plays key roles in protein interactions and stability. This study investigates the thermal stability of the FN3 domain from the thermophilic bacterium *Thermoanaerobacter tengcongensis*. The domains of the wild type and its triple mutant FN3 were simulated (Protein Data Bank ids: 7jgt and 7jgu, respectively), with a wild-type human analogue (Protein Data Bank id: 5kf4) as a control, using molecular dynamics (MD) with classical force field. The simulations were performed at 300, 350 and 400 K temperatures to show their impact on the molecular properties. Structural parameters were analyzed, including root mean square deviation (RMSD), root mean square fluctuations (RMSF), solvent accessible surface area (SASA), secondary structure assignment and hydrogen bond networks. The obtained results reveal that the thermophilic bacterial variants of the FN3 domain exhibit lower structural fluctuations, particularly in residues 10–20 and 50–60, compared to the human analogue. The bacterial FN3 mutant exhibited reduced stability compared to the wild type, highlighting the importance of hydrogen bonding network in ensuring thermal stability. These findings enhance our understanding of the molecular mechanisms underlying the stability and adaptation of extremophilic proteins to high temperatures.

Słowa kluczowe

thermophilic proteins, mesophilic proteins, extremophiles, FN3 domain, secondary structure, salt bridges, molecular dynamics, classical force fields, RMSD, RMSF, SASA

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