CALIFORNIA STATE SCIENCE FAIR
2007 PROJECT SUMMARY

Name(s)
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S0417

Project Title
Dancing Helices in Vacuum: A Computational Study of Peptide Molecular Dynamics

Abstract

Objectives/Goals
Biomolecules are not rigid; they fluctuate and participate in a variety of motions. A common protein or peptide secondary structure is an alpha-helix. Certain amino acids, like alanines, have propensities for alpha-helical structures. The objective of this study is to answer whether or not the length of a poly-alanine peptide affects its structural stability.

Methods/Materials
I have used computational tools to construct the following 5 polyalanine peptides of variable lengths. All peptides are perfect alpha-helices, because I fixed their backbone torsion angles to their theoretical values. All backbone hydrogen bonds are in place. The peptides are A5, A8, A11, A15, and A18, with 5, 8, 11, 15, and 18 alanines, comprising of 1-5 alpha-helical turns. I have performed molecular dynamics (MD) simulations in vacuum at 273K to study the unfolding of these peptides. The MD simulation for each peptide was 100 ps long. For the longest peptide, A18, an additional 1 ns simulation was performed. The software I used is DEEP VIEW for peptide design, VMD with NAMD interface for molecular dynamics, MOLMOL for analysis of MD trajectories.

Results
Structural analysis consists of calculations of hydrogen bonds and Ramachandran plots, using snapshots from the MD trajectories. The peptides A5, A8, and A11 unfold within 10 ps. A15 unfolds after 20 ps and A18 partially unfolds during 100 ps. The longer peptides unfold slower. The termini of the peptides unfold first. A18 shows that the unfolding is progressive from the end to the middle. During the 1 ns MD trajectory of A18, the alpha-helix unfolds and partially refolds.

Conclusions/Discussion
The longer peptides unfold slower, because they have larger number of hydrogen bonds. A18 has the largest number of hydrogen bonds and therefore unfolds slowest. The termini of the peptides unfold first, because the 4 first and 4 last amino acids have capability for only 1 backbone hydrogen bond each. The middle amino acids have capabilities for 2 backbone hydrogen bonds each. This is consistent with experimental data that suggest helices are stable in the middle and fraying at the termini. The longest peptide, A18, does not fully lose structure during the 1 ns of the MD trajectory. I have shown that peptides (and by extrapolation proteins in general) are dynamic entities, they fluctuate, their hydrogen bond patterns form and deform, and their structures partially unfold and refold.

Summary Statement
I have used computer simulation to demonstrate that peptides and proteins are dynamic.

Help Received
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