CALIFORNIA STATE SCIENCE FAIR
2005 PROJECT SUMMARY

Name(s)
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Project Number
S0599

Project Title
Stranding and Looping

Abstract

Objectives/Goals
I will test the hypothesis that nature prefers strands and helices in building biomolecules. I will also test if strands and helices are more stable structures than extended conformations.

Methods/Materials
I used a computer to make model peptides with repeating pentapeptide blocks of the type of [AAAAA](n) and [DAAAK](n), where n is the number of blocks; n=1-4. I modeled extended, strand, and helical structures. I measured and compared the stabilities of the peptides with and without energy minimization. I used the programs Insight II, IsisDraw, and DeepView.

Results
Examination of the potential energies, showed that helix is in general the most stable conformation, followed by strand, whereas the least stable is the extended conformation. As more amino acid blocks were added the gaps in the stabilities of helices, strands, and extended conformations become larger.

Conclusions/Discussion
Analysis of the individual potential energy terms for bond, angle, torsion, van der Waals, and electrostatic contributions, showed that the van der Waals term contributed the most to the increase in stability and to a lesser extend the electrostatic term. The [DAAAK](n) peptides were more stable than the [AAAAA](n) peptides, because of the formation of favorable anion-cation interaction between D, an acid, and K, a base.

Summary Statement
My project demonstrated that helices and strands are the preferred conformations for arranging amino acids in biomolecules.

Help Received
Father suggested the project and introduced me in molecular mechanics. Part of this work was performed at the University of California, Riverside under the supervision of Dr. Dimitrios Morikis. Mother helped me in gluing the project.