Protein Stability of a 21 Residue Alanine Based Peptide

Stough, Rusty [1,2]; Madura, Jeffry[3]; Asciutto, Eliana[4]

[1]*Bioenginerring and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh, Pittsburgh, PA*

[2]*Geneva College, Beaver Falls, PA*

[3]*Center for Computational Chemistry Duquesne University, Pittsburgh, PA*

[4]*Center for Computational Chemistry Duquesne University, Pittsburgh, PA*

Abstract

The central dogma of biochemistry has, for years, been how proteins go from a chain of amino acids to a three dimensional folded structure. The affects of ion interactions in the stability of proteins are studied here. In the body there are many different salts in solution, such as acetate, phosphate, and sulfate. It is well known that interactions with these salts cause affect protein stability, hence the structure depends on the environment. This study looks at the effects on stability of a short alanine based peptide in these salt solutions. The object was to find whether they would stabilize or destabilize the peptide.

Introduction

It is well known that alanine rich peptides form alpha-helices readily. The stability of which has been generally assumed to be because of the hydrophobicity of the side chains. Research into this field of study has been increasing in the recent years as many researchers are beginning to understand that this will help to solve the central dogma of biochemistry. Since this is a difficult task to perform in vitro it is useful, and gives much faster results, if the simulations are run in a computer.

In the past there has been much research in the fields of salt stabilization on peptides. The idea of salt bridges being a form of backbone stabilization has been examined in depth. Differing salt solutions have been studied thoroughly to determine their stabilizing affects. Sulfate has been shown to destabilize, while acetate and phosphate have been shown to stabilize. There are good and usable results from these experiments. However, more experimentation needs to be done and it will be through this experimentation that biochemists will be able to research the results from many different proteins in one salt solution and, at least in theory, be able to better understand how these salts affect proteins.

Throughout the years that it has been around, AMBER has been a useful tool in simulating molecular dynamics. The force fields that are in place help biochemists to solve problems.

Peptide Configurations

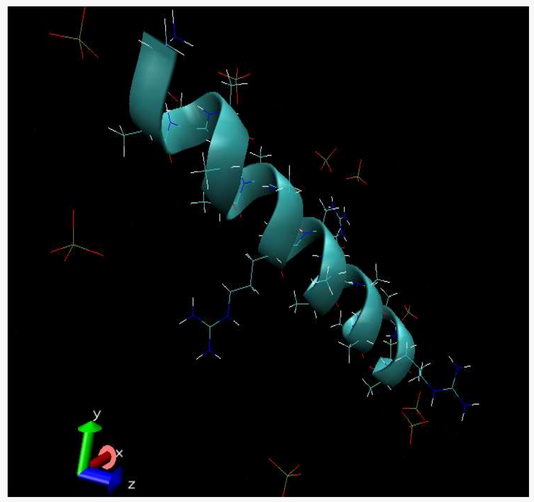


Figure 1: Peptide and Phosphate

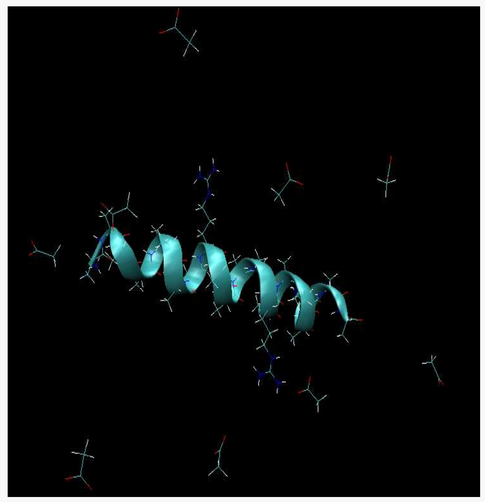
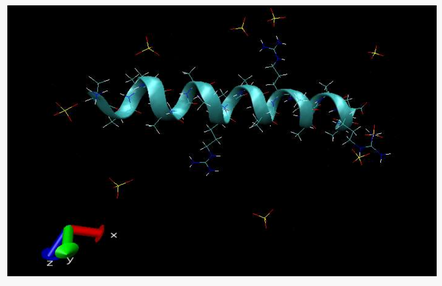
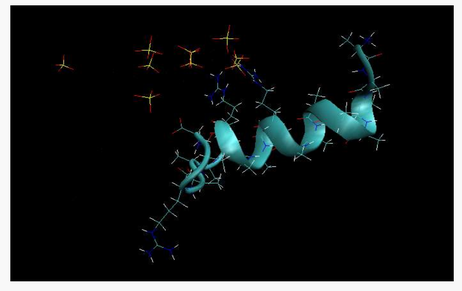


Figure 2: Peptide and acetate

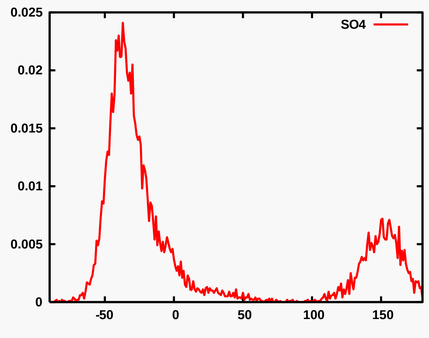
Sulfate Results



Initial Peptide and Salt Solution



After 14 nano seconds



- Psi plot of simulation
- Prefers alpha helix
- Only 1 nano second
- 70 nano seconds running

Future Research

- Signs of destabilization
- Running for 70 nano seconds
- Structure checked afterwards

Acknowledgements

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Dr. Jeffry D. Madura

Duquesne University

Dr. Eliana K. Asciutto

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