

## Mechanical Properties of Special DNA Sequences

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### Abstract

Diverse genetic diseases have been attributed to a presence of nucleotide repeat DNA sequences, the so-called microsatellites (MS). It is still unknown why MS cause these diseases. In this work we have investigated, through Molecular Dynamics simulations, how the presence of specific MS affect the DNA mechanical properties. Our preliminary results show that the presence of these repeats make the DNA “softer” to mechanical elongation under force deformation.

Key words: Deoxyribonucleic acid, Molecular Dynamics, Microsatellites.

### Introduction

The DNA is a macromolecule that carries all the genetic information for living things, from color eye to every biological instruction of our body. DNA is made of of several blocks named nucleotides. These blocks contain a phosphate group, a sugar group and one of 4 types of nitrogen bases: Adenine, Thymine, Guanine and Cytosine.

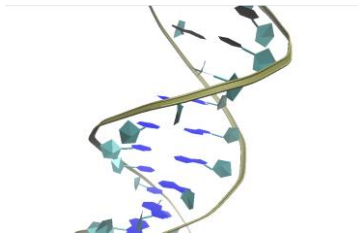


Image 1. Representation of a DNA segment.

The DNA replication is a very efficient process, but results in errors from time to time. These replication errors can result in the creation of microsatellites (MS), i. e., repeated sequences from 2 to 5 base pairs long. There is a great interest in the study of MS due to recent studies [1] showing a direct correlation between the presence of MS with some genetic diseases.

In this work we have investigated how specific sequences (AAG, for instance) affect the mechanical properties of the DNA molecule.

We considered DNA molecules containing 300 base pairs. We considered the cases of sequences from real human DNA and the ones generated containing diferent MS sequences, while keeping the total number of bases constant. and pulling with a constant force in each tip we analyzed the results.

These different DNA structures were subject to an externally applied force and the equilibrium DNA length calculated.

These calculations were carried out through molecular dynamics simulations using the NAMD [2] code coupled to the well-known CHARMM force field.

### Results and Discussion

In Figure 1 we present the results for human DNA and for structures containing 19 and 49 AAG repeats, respectively.

As we can see from this Figure, after a certain time of the simulations (~80 ps) the structures start to present distinct behaviors. The structures containing the repeats seems to be “softer” to mechanical elongation.

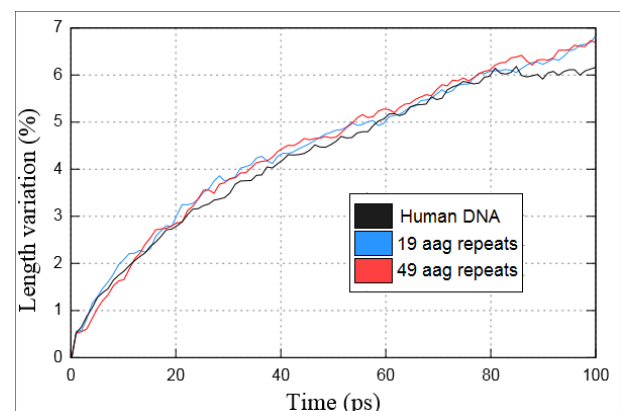


Image 2. Length variation of the DNA

### Conclusions

It is observed that the presence of MS make DNA “softer” to mechanical elongation under an externally applied force. Further studies are needed to confirm whether these results hold for structures containing a larger number of bases, as well as, which are the biological implications of these results.

### Acknowledgement

Work supported in part by the Brazilian Agencies CNPq and FAPESP.

<sup>1</sup>R. D. Wells, J. Biol. Chem. **271**, 2875 (1996).

<sup>2</sup>S. Plimpton, J. Comp. Phys. **117**, 1 (1995).