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Title: Effects of temperature on Nucleic Acids unzipping

Authors: Bharti, Naman Kumar (/jspui/browse?type=author&value=Bharti%2C+Naman+Kumar)

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Abstract:

This thesis deals with the molecular aspects of unzipping of Nucleic Acids using steered molecular dynamics computationally. In a human body or any living organism, this conversion of double strand to single strand process is very common in many biological processes. The unzipping of nucleic acids can also be studied experimentally using optical tweezers and AFM techniques but to get the idea of how these processes work without any experimental setup we use molecular dynamics technique. With this molecular dynamics technique we can model any kind of biological system to study the behavior of those microbiological system. In this work, we will be unzipping RNA and DNA with a hairpin using Steered Molecular Dynamics (SMD) in different environmental conditions. With different forces and pulling velocity the unzipping of nucleic acids was studied. And a comparative study between DNA & RNA and a DNA hairpin & without hairpin and DNA hairpin at room temperature & high temperature was also done.

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