

Abstract

Unzipping of Double Stranded DNA (dsDNA) into Single Stranded DNA (ssDNA) is a ubiquitous process which is central to many biological processes. In order to understand the dynamics and kinetics of these processes, Single molecule micromanipulation techniques has provided a new insight to understand these processes. These techniques include optical tweezers, atomic force microscopy (AFM) and micro niddle. In the present work, we use Steered Molecular Dynamic (SMD) to understand the dynamics. We used different solvation methods includes implicit and explicit solvation. In case of B-DNA dodecamer, A comparative study was done for different spring constant with different velocity and It is found that, at lower spring constant there are long pauses. Another study on DNA hairpin shows that, at high temperature it required less force than the low temperature. In comparison with implicit and explicit it was found that implicit shows better result than explicit. All of these are best explained in the next sections.