Weekly report

02/26/2012

Carolina

DNase I cleavage rate and its correlation with DNA parameters

Continuing the analysis of DNA parameters and their correlation with DNase I cleavage rate, here we take in consideration a new set of hexamers with different cleavage rates. In this new analysis though, we could not find the same correlation found between cleavage (for set1) and specific parameters such as phase, roll, and torsion angles alpha, gamma, epsil, delta and chi. As in the 2nd set the hexamers’ cleavage rates are not equally distributed between highest and lowest as in the 1st set, this might be affecting the correlation that we were previously seeing for the 1st set. To further understand the correlation between cleavage rate and DNA features we will extend our analysis to more hexamers with varying cleavage rates.

Studying p53 binding sites and setting new constrains for simulations

The idea here is to build new constraints for the MC so that we can adjust the DNA sequence to bind to the tetramer as a whole; while the regions to which the tetramer is more strongly bound to should not move as much, the central part of the DNA should be more flexible in order to accommodate the DNA and the tetramer. We will do that by restricting the region that can be occupied by the DNA based on the presence of the protein and distance between atoms in different nucleotides.
Papers:


Goals for this week

- Analyze new set of hexamers; get hexamers from previous simulations;
- MC simulations for p53 REs with constraints;