Weekly Report

Yan Lu

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1 Addition of p53 constraints

Added specific constraints for p53 in MC program and submitted jobs. There are totally 18 jobs which include:

- Using 3kmd’s distance parameters for both 3kmd and bax’s sequences
- Using bax’s distance parameters for both 3kmd and bax’s sequences.
- Without any constraints for both 3kmd and bax’s sequences.

So there are 6 sets and 3 independent simulations in each set. The distance parameters are defined as in Figure 1

2 Papers

1. Lee et al.[1] found that methylation induces tight wrapping of DNA around the histone core accompanied by a topology change by using FRET method (Figure 2).
   [What kind of topology change of the nucleosome DNA is not clear.]

2. Through single-molecule force experiments and simulation, Severin et al. [2] investigated the effects of methylation on strand separation of DNA, a crucial step in gene expression. The results show that mDNA has lower stacking energy and adopts a shorter, ordered zipper-like conformation with fewer bubbles shown in Figure 3
3kmd

g12 = 34.61, g13 = 49.49, g14 = 17.89, g23 = 17.37, g24 = 22.89, g34 = 34.01

c12 = 36.67, c13 = 50.35, c14 = 19.29, c23 = 18.42, c24 = 22.89, c34 = 36.60

g12 = 34.92, g13 = 30.12, g14 = 13.16, g23 = 13.33, g24 = 43.07, g34 = 34.54

c12 = 36.04, c13 = 30.21, c14 = 13.20, g23 = 13.45, g24 = 44.92, g34 = 35.73

bax

c12 = 34.61, c13 = 49.49, c14 = 17.89, c23 = 17.37, c24 = 22.89, c34 = 34.01

g12 = 34.92, g13 = 30.12, g14 = 13.16, g23 = 13.33, g24 = 43.07, g34 = 34.54

c12 = 36.04, c13 = 30.21, c14 = 13.20, g23 = 13.45, g24 = 44.92, g34 = 35.73

Figure 1: Definition of distances for p53.
References


Figure 2: Shows methylation induces tight wrapping of DNA around the histone core. The pale-colored histograms in (B) and (D) are replicas of the histograms in (A) and (C), respectively[1].
Figure 3: (a) Stacking energy versus extension curves of 15 trajectories of DNA pulled at 10 Å/ns velocity. (b) Stacking energy versus extension data from two 90-ns-long constant force (F=200 pN) simulations. The results show that mDNA has lower stacking energy and adopts a shorter, ordered zipper-like conformation with fewer bubbles (left), while nDNA adopts a longer, zipper-like conformation with more bubbles (right). Orange circles indicate the positions of methylated cytosines [2].