

Molecular and Neural Computation (CSE P 590B)

Homework 1

1. DNA Computation (NuPACK)

For problems 1 and 2, you will use the NuPACK Analysis tool: <http://nupack.org>.

Suppose you have 4 strands of DNA:

P1: CTATCATCACACATCTATAACAACCACTTACTTCTTC

L1: GGATAGATGAAGAAGTAAGTGGTTGTATAGATGTGTGATGATAGTAGTGATG

T1: CATCACTACTATCATCACACATCTAT

T2: ACAACCACTTACTTCTTCATCTATCC

Initially, P1 and L1 are mixed in a test tube at 25C where the initial concentration of P1 is 30 nM, the initial concentration of L1 is 30 nM, the solution contains Na⁺ at a concentration of 0.05 M, and Mg²⁺ at a concentration of 0.0115 M.

- a) At equilibrium, what complexes are at the greatest concentration? Include the equilibrium concentration and the MFE structure that NuPACK predicts.

The mixture from part (a) along with strands T1 and T2 form an input/output system where initial concentrations of T1 and T2 are inputs, and the concentration of P1 at equilibrium is an output. For the following initial concentrations of inputs T1 and T2, what complexes are at the greatest concentration at equilibrium? (For each system use the same initial concentrations of P1, L1, Na⁺, and Mg²⁺ as in part (a).)

- b) T1 at 0 nM, T2 at 20 nM
T1 at 10 nM, T2 at 20nM
T1 at 20 nM, T2 at 0 nM
T1 at 20 nM, T1 at 10 nM
T1 at 20 nM, T2 at 20nM

- c) What does this input/output system do? Describe (in text and/or figures) how you think it works.

2. Designing Secondary Structure in DNA (NuPACK)

You may find it useful in this problem to use the NuPACK Design tool:

<http://nupack.org/design>. Your solutions should fold in NuPACK at 20C with Na⁺ concentration of 1 M, and Mg²⁺ concentration of 0 M.

- a) Make a snowman. That is, design a sequence for a single strand of DNA (no more than 50 bases long), that folds into a secondary structure that has three "loops" of increasing size that looks somewhat like the outline of a snowman. Analyze your structure in NuPACK (make sure to set the "Maximum complex size" to be

at least 2). Include the relative concentrations of the most likely complexes and their MFE structure.

- b) Design three sequences of DNA that fold into the following shape with high probability. Each sequence should be no more than 20 bases long. Again, analyze your structure in NuPACK (make sure to set the “Maximum complex size” to be at least 3), and include relative concentrations of the most likely complexes and their MFE structure.

