CompSci 590 HW2

Molecular Assembly and Computation

(Question one through Question seven)

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Problem 1: Enzyme-based DNA Computing

Design a set of enzyme-based DNA logic gates (AND gate and OR gate) with emphasis on:

• (a) leak reduction, explain how you aim to design your gates to be leakless
Answer: *leak*: incorrect signal production.

• (b) scalability which means that the gates should be able to work together as a circuit. You are allowed to use any enzyme.

Cite: 1 Design of enzyme-interfaced DNA logic operations (AND, OR and INHIBIT) with an assaying application for single-base mismatch
2 Leakless DNA Strand Displacement Systems Fig 4 and Fig 5

Problem 2: Enzyme-based DNA Computing

- (2a) Using class materials as well as literature search, find two different deoxyribozymes (DNAzymes) and describe in detail their properties. Using the DNAzymes you have chosen, construct a half-adder and a full-adder. Please cite all sources you have used to answer this question.

cite: `http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.87.1221&rep=rep1&type=pdf`

- (2b) Using class materials as well as literature search, construct hairpin-based OR, AND, and XOR gates. Describe an implementation of ripple-carry adder with the gates you have answered from the previous part. Please cite all sources you have used to answer this question.

Problem 3: Hybridization-based DNA Computing

- (3a) Read the article: `http://science.sciencemag.org/content/332/6034/1196andwriteaparagraphofsummary.\`
- (3b) Design a DNA digital circuit to compute square roots for 2-bit numbers using seesaw gates.

- (3c) Simulate your circuit using LBS (Language for Biological Systems) in Visual GEC:

LBS (Language for Biological Systems): see `http://homepages.inf.ed.ac.uk/gdp/publications/Lang_Bio_Sys_Design_Spec.pdf`

Visual GEC: see `http://lepton.research.microsoft.com/webgec/`

Problem 4: (DNA-based Molecular Robotics)

- (4a) Every robotics system requires fuel to function. List the different types of fuel used currently in DNA robotic reactions and mention at least 3 examples (with references) for each.

- (4b) What role does concentration play in fueling robotic motion? Explain this for each of the different types of fuel.

- (4c) List 3 different ways of observing/reporting/confirming robotic motion (fluorescence, imaging, gel) and provide 3 examples (with references) on each.

- (4d) Summarize an example DNAzyne-based or hybridization based robotics demonstration from 2014 onwards, and argue why you consider it to be so.

Problem 5: Enzyme based DNA Robotics:

DNA Robotics is the study of designing DNA systems that can perform conformational changes/ display locomotion. In order to perform any change, energy is required. Let us take the example of a DNA walker - "A Unidirectional DNA Walker That Moves Autonomously along a Track" (See `https://users.cs.duke.edu/~reif/paper/harish/NanoRobotics/NanoRobotics.pdf` for an easier explanation of the article).

- (5a) What is the source of energy for this locomotion. Give the chemical reaction that is involved in this system that releases energy.

- (5b) Is this reaction reversible, i.e. can the walker move in the reverse direction?

- (5c) List all the enzymes involved in this particular walker, and the DNA recognition sequences that they cut.

- (5d) Currently this design is limited to 2 steps. Can this design be extended to 4 steps. If so, how? Will you need more enzymes?

Problem 6: DNAZyme based DNA Robotics:

- (6a) Read the article. Molecular robots guided by prescriptive landscapes.

- (6b) What is the difference between a DNAzyme and an enzyme. In one sentence.

- (6c) What is the source of energy for this locomotion. Give the chemical reaction that is involved in this system that releases energy.

- (6d) What type of molecule is cleaved by the DNAzyme?

Problem 7: DNA-based Molecular Robotics Design

- Design an arbitrary track, and a simple DNAzyme-based or hybridization-based DNA robotic system which can move along that track. You can use any sort of track. Submit the design to a simulation software (using NUPACK or canDo, for example, or both) with a simulation of two or more steps of locomotion, and provide the results of the simulation .