**4bm Computer Simulation Studies of Pattern Recognition in Biomimetic Polymers**

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Abstract: The overall aim of my research has been to understand the underlying molecular phenomena governing recognition in numerous biological processes such as transmembrane signaling, pathogen-host interactions, viral-inhibition, etc. Specifically, I have used computer simulation to study the thermodynamics of recognition and selective adsorption of biopolymer sequences. I will briefly present my work on the following topics:

1. Designing pattern recognition surfaces for selective adsorption of copolymer sequences : Most of the theoretical work in the area of the pattern recognition by biomimetic polymers has focussed on keeping the pattern on the heterogeneous surface fixed and allowing different types of copolymers to adsorb on the surface to determine the characteristics of the copolymer that can "recognize" the surface pattern. However, the question of how to design optimal surfaces or what pattern the surfaces should have for recognizing specific monomer sequences in copolymers, had not been answered yet. To address this issue, we have developed a novel simulation method to design surfaces for recognizing specific monomer sequences in copolymers [1]. The order parameter characterizing the surface pattern, and the surface selectivity are determined as a function of polymer-surface and polymer-polymer interactions, and the blockiness of the monomer sequence. The highlight of this work is that the designed surfaces recognize specific monomer sequences with higher selectivity than the standard checkboard surfaces of sizes commensurate with the monomer sequence. This work provides the foundation for future work in understanding many biological processes that rely on pattern recognition, such as transmembrane signaling, pathogen-host interactions, viral-inhibition, etc.

2. Molecular recognition in model DNA microarrays : DNA microarrays has been widely adopted by the scientific community for a variety of applications to reconstruct the metabolic pathways for cell operation, to identify genes that are differentially expressed in healthy versus diseased cells, etc. In order to improve performance and to design next generation microarrays there is a need for a fundamental understanding of the interplay between the various factors that affect microarray performance. To gain such a fundamental understanding we study the thermodynamics and the kinetics of hybridization of single stranded "target" genes in solution with complimentary immobilized "probe" DNA molecules on a microarray surface using a coarse-grained lattice model. We use Monte Carlo simulations to examine how various parameters affect the extent of hybridization and the kinetics of the hybridization process. This work should give a fairly broad physical picture of molecular recognition in DNA microarrays and eventually provide a set of general guidelines for maximizing microarray sensitivity and specificity.

References: [1] A. Jayaraman, C. K. Hall, J. Genzer, "Designing pattern-recognition surfaces for selective adsorption of copolymer sequences using lattice Monte Carlo simulation", Physical Review Letters 94 (7) 078103 (2005)