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Structure and Sequence Search on Aptamer-Protein Docking JIAJIE XIAO, KEITH BONIN, MARTIN GUTHOLD, FREDDIE SALSBURY, Wake Forest University — Interactions between proteins and deoxyribonucleic acid (DNA) play a significant role in the living systems, especially through gene regulation. However, short nucleic acids sequences (aptamers) with specific binding affinity to specific proteins exhibit clinical potential as therapeutics. Our capillary and gel electrophoresis selection experiments show that specific sequences of aptamers can be selected that bind specific proteins. Computationally, given the experimentally-determined structure and sequence of a thrombin-binding aptamer, we can successfully dock the aptamer onto thrombin in agreement with experimental structures of the complex. In order to further study the conformational flexibility of this thrombin-binding aptamer and to potentially develop a predictive computational model of aptamer-binding, we use GPU-enabled molecular dynamics simulations to both examine the conformational flexibility of the aptamer in the absence of binding to thrombin, and to determine our ability to fold an aptamer. This study should help further de-novo predictions of aptamer sequences by enabling the study of structural and sequence-dependent effects on aptamer-protein docking specificity.

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