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Design of ligand binding proteins faces several challenges including sampling of the enormous possible orientations of the ligand with respect to the protein, the large conformational and the sequence space of the protein pocket, and the difficulties in accurately estimating the binding free energies during the course of design.
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The ability to design proteins with high affinity and selectivity for any given small molecule would have numerous applications in biosensing, diagnostics, and therapeutics, and is a rigorous test of our understanding of the physicochemical principles that govern molecular recognition phenomena
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The ability to design novel small-molecule binding sites in proteins is a stringent test of our understanding of the principles of molecular recognition, and would have many practical applications.
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Custom-designed ligand-binding proteins with novel functions hold the potential for numerous applications. In recent years, the developments of computational methods together with high-throughput
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Computational design of ligand-binding proteins with high affinity and selectivity Christine E. Tinberg 1 , Sagar D. Khare 1 , Jiyi Dou 2,3 , Lindsey Doyle 4 , Jorgen W. Nelson 5 , Alberto Schena 6 , Wojciech Dankowski 7 ,
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This volume provides a collection of protocols and approaches for the creation of novel ligand binding proteins, compiled and described by many of today's leaders in the field of protein
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However, a particular aspect of computational protein design that has proved more difficult is the design of protein ligand interfaces, particularly the design of proteins

capable of tightly binding small molecules and peptides (Hayden, 2009; Schreier et al., 2009a).