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Engineering protein structure and function with computational protein design JEFFERY SAVEN, University of Pennsylvania — Understanding molecular folding has important applications to understanding biology and to developing new therapeutics and new materials. Protein design also opens new ways to probe the determinants of folding and to facilitate the study of proteins. Such design is complicated, however, by the conformational complexity of proteins and by the large numbers of possible sequences. Recent computational methods for identifying the properties of amino acid sequences likely to fold to a given three-dimensional structure will be presented. Several examples of structures so designed, which have been experimentally synthesized and characterized, will be presented.

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