

From sequence to structure, to function, and back again: Integrating knowledge-based approaches with physical intuitions for protein folding, binding, and design

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Abstract

Most biological activities are directed and/or regulated by proteins made of a gene-specified sequence of 20 amino-acid residue types. As a result, function or malfunction of specific proteins is responsible for almost all diseases. Proteins perform their function through their unique, self-assembled (folded) three-dimensional structures and through their specific binding to small molecules, to DNA/RNA (e.g. transcription factors that regulate gene expressions), or to other proteins (e.g. molecular recognition in signal transduction). Thus, how to predict the structure of a protein from its amino-acid sequence, discover the function from its structure and, then, design the sequence from its function or structure are the most essential problems in structural biology. In this poster, we will illustrate how the coupling of physical intuitions with learning from structural databases can go a long way toward untangling the complex relation between sequence, structure and function of proteins.