Emergence of Complexity in Protein Functions and Metabolic Networks
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In modern organisms proteins perform a majority of cellular functions, such as chemical catalysis, energy transduction and transport of material across cell walls. Although great strides have been made towards understanding protein evolution, a meaningful extrapolation from contemporary proteins to their earliest ancestors is virtually impossible. In an alternative approach, the origin of water-soluble proteins was probed through the synthesis of very large libraries of random amino acid sequences and subsequently subjecting them to in vitro evolution. In combination with computer modeling and simulations, these experiments allow us to address a number of fundamental questions about the origins of proteins. Can functionality emerge from random sequences of proteins? How did the initial repertoire of functional proteins diversify to facilitate new functions? Did this diversification proceed primarily through drawing novel functionalities from random sequences or through evolution of already existing proto-enzymes? Did protein evolution start from a pool of proteins defined by a 'frozen accident' and other collections of proteins could start a different evolutionary pathway? Although we do not have definitive answers to these questions, important clues have been uncovered.

Considerable progress has been also achieved in understanding the origins of membrane proteins. We will address this issue in the example of ion channels - proteins that mediate transport of ions across cell walls. Remarkably, despite overall complexity of these proteins in contemporary cells, their structural motifs are quite simple, with α-helices being most common. By combining results of experimental and computer simulation studies on synthetic models and simple, natural channels, I will show that, even though architectures of membrane proteins are not nearly as diverse as those of water-soluble proteins, they are sufficiently flexible to adapt readily to the functional demands arising during evolution.

A critical step in the transition from inanimate to animate matter was self-organization of catalyzed chemical reactions into metabolic pathways and networks. Using computer simulations of biochemically motivated models of protocellular reproduction and evolution I will show that the highly stochastic processes leading to the formation of metabolic networks could have led to a largely deterministic outcome. I will further demonstrate that such concepts as speciation and fitness to the environment, developed in the context of genomic evolution, also held in the absence of a genome. Finally, I will discuss implications of these results for the universality of life-forming processes.