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Editorial

Systems Biology: Roles for Thermodynamics and Catalysis

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EDITORIAL

In mammalian biology, the primary task has switched to understanding the functional interactions between molecules in cells and tissues, as well as how specific molecular components work as modules. This enormous problem is addressed by systems biology, which focuses on synthesizing functional linkages in the form of networks and pathways. The networks, in general, describe the interactions between molecules in a cell as reactions, activation, or inhibitory events. Spatial and temporal signals flowing across intracellular signaling pathways decipher the specificity of such biological responses. Network analysis techniques decode functional insights into the complicated interactions between stimuli, cellular responses, and cell fate by encoding quantitative relationships.

Only three-dimensional structures, which reveal atomic data about the specificity of binding and molecular recognition, can provide a thorough understanding of how molecules interact. Because of the difficulties in determining macromolecular (protein-protein and protein-nucleic acid) interfaces and dealing with large protein complexes, structural biology has largely remained limited in terms of informing systems biology. New crystal structure determination techniques, on the other hand, have recently evolved to predict and model the structures of interacting proteins. Improvements in overexpression and purification procedures to obtain sufficient material for structural analysis, the ability to express complex subunits in model organisms, and crystallization techniques and synchrotron radiation facilities to use smaller sample amounts to solve problems are among them.

Cryoelectron microscopy, for example, is used to recreate structures of huge complexes at lower resolution with considerably less material. A lot of work has gone into compiling comprehensive listings of protein-protein interactions. Although other experimental methods such as chemical cross linking, chemical foot printing, protein arrays, fluorescence resonance energy transfer, and fluorescence cross correlation spectroscopy are becoming more popular, the yeast two-hybrid system and affinity purification methodologies remain the most widely used systems. Despite these gains, there is still a significant gap between the number of inferred complexes and those for which 3-dimensional structures are accessible.

Multiscale computer modeling, which applies fundamental principles of thermodynamics and catalysis to systems at the Nano to micro-scale, can help researchers better understand chemical complexes and how they spread at the cellular signaling scale. The goal of multistate modeling is to bridge the structural and systems biology scales in order to understand the consequences of macromolecular structure perturbations on downstream signaling events triggered by multiprotein complexes. Because the stability of biological systems depends on the efficient flow of information across various geographical and temporal dimensions, multiscale modeling approaches are an effective way to bridge the scales and provide more insights than a single scale could provide.

Protein-protein interactions can be predicted computationally, allowing high-throughput studies to be supplemented. On the one hand, statistical approaches are based on entire genome sequence comparisons and more established complementarity criteria, as illustrated by the substantial literature in yeast genetics, or on co-evolution patterns across multiple species. Interacting protein structures can also be modeled computationally using homology modeling (assuming structures for relevant homologous proteins have already been determined). In the lack of known structural information, domain or motif-based modeling methods can be used. Several domain-domain and domain-motif interactions have been predicted using these methods. On the other hand, computational chemistry methodologies based on the potential energy (or force-field) of molecular interactions to predict atomic details for a pair of interacting proteins are also available, based on principles of statistical mechanics and thermodynamics.

On the basis of form or electrostatic complementarity, or directly on the underlying free energy landscape mediating the protein surfaces, docking algorithms seek to determine the best-docked complex. The organized assembly of macromolecular complexes is difficult to capture under most experimental settings, hence building accurate macromolecular complexes remains a challenge. New hybrid approaches for predicting macromolecular complex structure that integrate various scales

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are becoming more widely available. One approach to molecular complex prediction is hybrid multiscale approaches, which integrate numerous lower resolution techniques to build atomic models of protein complexes. These hybrid techniques, which may include X-ray crystallography, cross-linking investigations, and cry electron microscopy, allow researchers to combine the accuracy of atomic level models with the computing speed of coarse grained models.