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Opinion Article

Role of Protein-Protein Interaction in High-Complexity Reactions

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DESCRIPTION

Complex wirings in Protein-Protein Interaction (PPI) networks precisely modulate the inner workings of the circuits that underpin cell life. Their proper or incorrect regulation is inextricably related to cell evolution towards normal or disease states. Because PPIs are involved in so many different aspects of cellular function, it's no surprise that they've been focus of extensive research in recent years. Understanding protein-protein recognition and binding necessitates shedding light on regulatory processes as well as expanding their understanding of the relationships between protein sequences, structure, and interactions. In practice, their ability to master PPIs could be critical in the areas of medicinal chemistry, chemical and synthetic biology. Indeed, there may be space not only for new strategies targeted at rewiring signalling pathways for synthetic biology, but also for the development of new molecules against complex or yet undragged targets for diagnostic and therapeutic purposes.

In general, PPIs are a type of high-complexity interaction. Structural and biophysical studies have revealed that the characteristics of the regions involved in interactions with other partners are diverse and multifaceted contact surfaces may be larger than those involved in protein-small molecule interactions; they are often flat and lack the grooves and crevices that small molecules engage in, and they are highly dynamic to favour adaptation to alternative binding partners. Mutational studies have revealed that only a subset of interface residues add to the binding partners' affinity. Flexible peptides selected by High-Throughput Screening (HTS) techniques (such as phage display or large library screenings) have shown the ability to outcompete the natural partner by adapting to the interaction surface in the context of targeting interface plasticity. Similarly, HTS of small molecules against biochemically reconstituted complexes has resulted in the discovery of useful compounds with phenotypic effects when evaluated in cells.

Instead of directly monitoring physical interaction, researchers set out to characterise the functional effects of inhibiting a specific class of PPIs as a surrogate for binding measurement in this instance. This is an intriguing example of using HTS methods to find modulators of PPI networks, highlighting the importance of approaching challenging PPIs with caution, such as those characterised by weak or transient interactions and for which classical HTS-based detection is ineffective.

These facts vividly depict a scenario in which many aspects of protein-protein interactions have been successfully investigated. Despite this sophistication and progress, no experimental technique can predict at the atomic level what makes a protein surface interact, or define rules for the design of new molecular entities with applications in chemical biology or drug development. They have little option to use theoretical and computational approaches to address these issues.

Molecular Dynamics (MD) simulations are an excellent tool for characterising both the networks of interactions and the range of alternative states that can decide whether a protein surface is truly an interacting one, as well as the dynamics of molecular recognition processes with binding partners. MD simulations can be combined with quantum calculations in some instances to explain complex reactive processes at the root of downstream recognition events. In general, framework involves using computational results to develop and test active chemical tools to probe a specific PPI. Such chemical probes are, in fact, direct products of our ability to understand and imitate the determinants of an interaction: in this sense, they are intended to target and perturb a specific area.

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