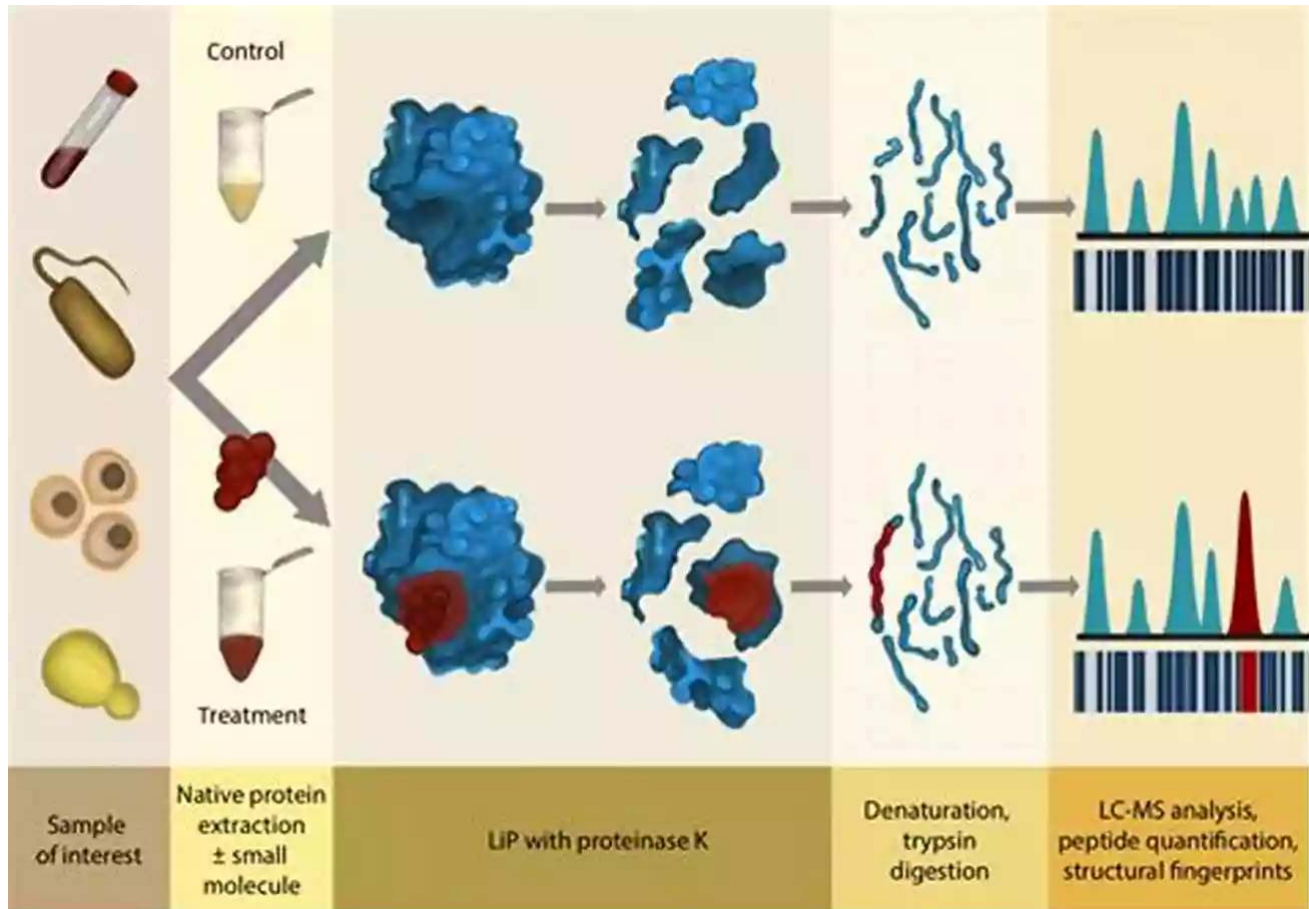


Targeting Protein-Protein Interactions By Small Molecules

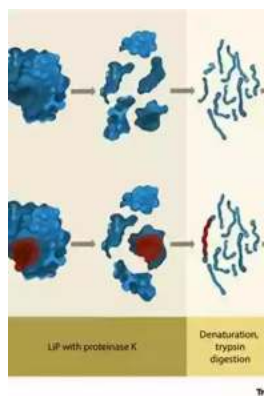


Trends in Biochemical Sciences

Protein-protein interactions play a crucial role in various cellular processes. These interactions are responsible for the formation of protein complexes, which are essential for the proper functioning of cells. When protein-protein interactions go awry, it can lead to various diseases and disorders. Therefore, understanding and targeting these interactions by small molecules has gained significant attention in the field of drug discovery.

Why Target Protein-Protein Interactions?

Traditional drug discovery approaches have mainly focused on designing small molecules that inhibit the activity of individual proteins. However, many diseases involve dysregulation of protein-protein interactions, rather than the activity of a single protein. Targeting protein-protein interactions offers a promising avenue for developing novel therapeutics that can modulate these interactions and restore normal cellular function.



Targeting Protein-Protein Interactions by Small

Molecules by David Brennan(1st ed. 2018 Edition, Kindle Edition)

★★★★☆ 4.3 out of 5

Language : English

File size : 13358 KB

Text-to-Speech : Enabled

Screen Reader : Supported

Enhanced typesetting : Enabled

Print length : 535 pages



The Challenges of Targeting Protein-Protein Interactions

Targeting protein-protein interactions presents several challenges due to the nature of these interactions. Protein surfaces involved in interactions are often large, flat, and devoid of deep pockets, making it difficult for small molecules to bind with high affinity and specificity. Additionally, protein-protein interfaces are typically dynamic, with conformational flexibility, further complicating the design of small molecules to disrupt these interactions. These challenges demand innovative approaches to develop successful inhibitors.

Strategies for Targeting Protein-Protein Interactions

Over the past decade, several strategies have emerged for targeting protein-protein interactions. One approach involves designing small molecules that mimic the structural features of one of the interacting proteins. These molecules can act as competitors, blocking the interaction between the two proteins. Another strategy focuses on disrupting critical protein-protein interface residues using computational methods and structure-based design. This approach utilizes the three-dimensional structure of the interacting proteins to identify potential binding pockets and design tailored inhibitors.

Another promising strategy is fragment-based drug discovery. This approach involves screening libraries of small molecule fragments for binding to the protein-protein interface. Once identified, these fragments can be further optimized and expanded to develop high-affinity inhibitors. Moreover, advances in high-throughput screening techniques and computational modeling have significantly contributed to the development of small molecule inhibitors that specifically target protein-protein interactions.

Applications of Targeting Protein-Protein Interactions

The ability to target protein-protein interactions holds immense potential for the development of therapeutics against various diseases. Examples include cancer, where the dysregulation of protein-protein interactions contributes to uncontrolled cell growth and metastasis. By designing small molecules that selectively disrupt specific interactions involved in cancer pathways, it may be possible to inhibit tumor growth and improve patient outcomes.

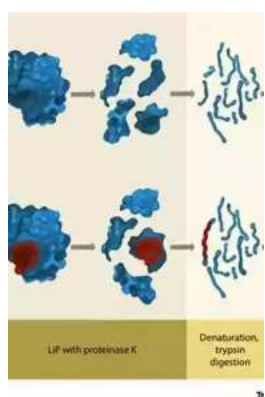
Targeting protein-protein interactions is also crucial in the treatment of infectious diseases. Many pathogens exploit protein-protein interactions with host proteins to establish infection and evade host immune responses. Developing small molecule inhibitors that disrupt these interactions can hinder pathogen survival

and replication, leading to the development of effective antiviral and antibacterial drugs.

The Future of Targeting Protein-Protein Interactions

As our knowledge of protein-protein interactions continues to expand, so does the potential for developing small molecule therapeutics that specifically target these interactions. Advances in computational methods, structural biology, and chemical synthesis techniques are accelerating the discovery and optimization of inhibitors against challenging protein-protein interfaces. The increasing availability of high-quality protein-protein interaction databases and computational tools further supports the design of tailored small molecules.

, targeting protein-protein interactions by small molecules has emerged as a promising strategy for drug discovery. It offers the potential to develop highly specific and effective therapeutics against diseases where dysregulated protein-protein interactions are involved. Although challenges remain, ongoing research and technological advancements are paving the way for the development of novel drugs that modulate protein-protein interactions and provide new treatment options for various diseases.



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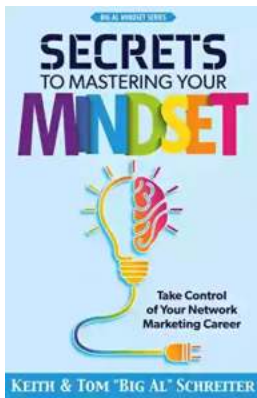
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This book comprehensively reviews the state-of-the-art strategies developed for protein-protein interaction (PPI) inhibitors, and highlights the success stories in new drug discovery and development. Consisting of two parts with twelve chapters, it demonstrates the design strategies and case studies of small molecule PPI inhibitors. The first part discusses various discovery strategies for small molecule PPI inhibitors, such as high throughput screening, hot spot-based design, computational approaches, and fragment-based design. The second part presents recent advances in small molecule inhibitors, focusing on clinical candidates and new PPI targets. This book has broad appeal and is of significant interest to the pharmaceutical science and medicinal chemistry communities.



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