Structure-based Design of Drugs and Other Bioactive Molecules: Tools and Strategies

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Drug design is a complex, challenging and innovative research area. Structure-based molecular design has transformed the drug discovery approach in modern medicine. Traditionally, focus has been placed on computational, structural or synthetic methods only in isolation. This one-of-akind guide integrates all three skill sets for a complete picture of contemporary structure-based design.

This practical approach provides the tools to develop a high-affinity ligand with drug-like properties for a given drug target for which a high-resolution structure exists. The authors use numerous examples of recently developed drugs to present "best practice" methods in structurebased drug design with both newcomers and practicing researchers in mind. By way of a carefully balanced mix of theoretical background and case studies from medicinal chemistry applications, readers will quickly and efficiently master the basic skills of successful drug design.

This book is aimed at new and active medicinal chemists, biochemists, pharmacologists, natural product chemists and those working in drug discovery in the pharmaceutical industry. It is highly recommended as a desk reference to guide students in medicinal and chemical sciences as well as to aid researchers engaged in drug design today.

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