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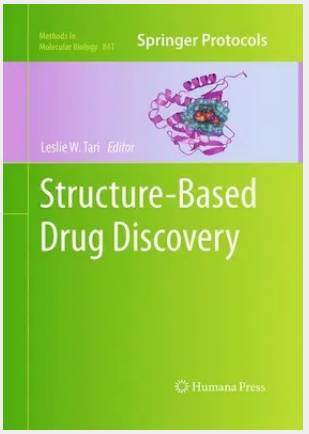
Structure-Based Drug Discovery



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The last decade has seen the confluence of several enabling technologies that have allowed protein crystallographic methods to live up to their true potential. Taken together, the numerous recent advances have made it possible to tackle difficult biological targets with a high probability of success: intact bacterial ribosomes have been structurally elucidated, as well as eukaryotic trans-membrane proteins like the potassium channel and GPCRs. It is now possible for medicinal chemists to have access to structural information on their latest small molecule candidates bound to the therapeutic target within days of compound synthesis, allowing structure guided ligand optimization to occur in "real time". *Structure-Based Drug Discovery* presents an array of methods used to generate crystal structures of biological macromolecules, how to leverage the structural information to design novel ligands anew , and how to iteratively optimize hits and convert them to leads. Written in the successful *Methods in Molecular Biology*™ series format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible protocols, and notes on troubleshooting and avoiding known pitfalls.

Authoritative and easily accessible, *Structure-Based Drug Discovery* aims to provide scientists interested in adding SBDD to their arsenal of drug discovery methods with well-honed, up-to-date methodologies.

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