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5 The Drug Design Process for a Known Protein Target; 5.1 The Structure-Based Design Process; 5.2 Initial Hits; 5.3 Compound Refinement; 5.4 ADMET; 5.5 Drug Resistance; Bibliography; 6 The Drug Design Process for an Unknown Target; 6.1 The Ligand-Based Design Process; 6.2 Initial Hits; 6.3 Compound Refinement; 6.4 ADMET; Bibliography; 7 Drug Design for Other Targets; 7.1 DNA Binding; 7.2 RNA as a Target; 7.3 Allosteric Sites; 7.4 Receptor Targets; 7.5 Steroids; 7.6 Targets inside Cells; 7.7 Targets within the Central Nervous System; 7.8 Irreversibly Binding Inhibitors
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9.2.2 Step 2: Alignment between the Unknown and the Template; 9.2.3 Step 3: Manual Adjustments to the Alignment; 9.2.4 Step 4: Replace Template Side Chains with Model Side Chains; 9.2.5 Step 5: Adjust Model for Insertions and Deletions; 9.2.6 Step 6: Optimization of the Model; 9.2.7 Step 7: Model Validation; 9.2.8 Step 8: If Errors are Found, Iterate Back to Previous Steps; 9.3 Reliability of Results; Bibliography; 10 Molecular Mechanics; 10.1 A Really Brief Introduction to Molecular Mechanics; 10.2 Force Fields for Drug Design; Bibliography; 11 Protein Folding; 11.1 The Difficulty of the Problem

Sommario/riassunto

Helps you choose the right computational tools and techniques to meet your drug design goals Computational Drug Design covers all of the major computational drug design techniques in use today, focusing on the process that pharmaceutical chemists employ to design a new drug molecule. The discussions of which computational tools to use and when and how to use them are all based on typical pharmaceutical industry drug design processes. Following an introduction, the book is divided into three parts: Part One, The Drug Design Process, sets forth a variety of design processes