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Nota di contenuto

Structure-based Design of Drugs and Other Bioactive Molecules: Tools and Strategies; Contents; Preface; 1 From Traditional Medicine to Modern Drugs: Historical Perspective of Structure-Based Drug Design; 1.1 Introduction; 1.2 Drug Discovery During 1928-1980; 1.3 The Beginning of Structure-Based Drug Design; 1.4 Conclusions; References; Part One: Concepts, Tools, Ligands, and Scaffolds for Structure-Based Design of Inhibitors; 2 Design of Inhibitors of Aspartic Acid Proteases; 2.1 Introduction; 2.2 Design of Peptidomimetic Inhibitors of Aspartic Acid Proteases
2.3 Design of Statine-Based Inhibitors
2.4 Design of Hydroxyethylene Isostere-Based Inhibitors; 2.5 Design of Inhibitors with Hydroxyethylamine Isosteres; 2.5.1 Synthesis of Optically Active -Aminoalkyl Epoxide; 2.6 Design of (Hydroxyethyl)urea-Based Inhibitors; 2.7 (Hydroxyethyl)sulfonamide-Based Inhibitors; 2.8 Design of Heterocyclic/Nonpeptidomimetic Aspartic Acid Protease Inhibitors; 2.8.1 Hydroxycoumarin- and Hydroxypyron- Based Inhibitors; 2.8.2 Design of Substituted Piperidine-Based Inhibitors; 2.8.3 Design of Diaminopyrimidine-Based Inhibitors
2.8.4 Design of Acyl Guanidine-Based Inhibitors
2.8.5 Design of Aminopyridine-Based Inhibitors; 2.8.6 Design of Aminoimidazole- and Aminohydantoin-Based Inhibitors; 2.9 Conclusions; References; 3 Design of Serine Protease Inhibitors; 3.1 Introduction; 3.2 Catalytic Mechanism of Serine Protease; 3.3 Types of Serine Protease Inhibitors; 3.4 Halomethyl Ketone-Based Inhibitors; 3.5 Diphenyl Phosphonate-Based Inhibitors; 3.6 Trifluoromethyl Ketone Based Inhibitors; 3.6.1 Synthesis of Trifluoromethyl Ketones; 3.7 Peptidyl Boronic Acid-Based Inhibitors
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3.8 Peptidyl -Ketoamide- and -Ketoheterocycle-Based Inhibitors; 3.8.1 Synthesis of -Ketoamide and -Ketoheterocyclic Templates; 3.9 Design of Serine Protease Inhibitors Based Upon Heterocycles; 3.9.1 Isocoumarin-Derived Irreversible Inhibitors; 3.9.2 -Lactam-Derived Irreversible Inhibitors; 3.10 Reversible/Noncovalent Inhibitors; 3.11 Conclusions; References; 4 Design of Proteasome Inhibitors; 4.1 Introduction; 4.2 Catalytic Mechanism of 20S Proteasome; 4.3 Proteasome Inhibitors; 4.3.1 Development of Boronate Proteasome Inhibitors
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6.3 Design of Inhibitors of Tumor Necrosis Factor--Converting Enzymes

Sommario/riassunto

In contrast to previous texts focusing on either computational, structural or synthetic methods, this one-of-a-kind guide integrates all three skill sets for a complete picture of contemporary structure-based design. As a result, this practical book demonstrates how to develop a high-affinity ligand with drug-like properties for any given drug target for which a high-resolution structure exists. The authors, both of whom have successfully designed drug-like molecules that were later developed into marketed drugs, use numerous examples of recently developed drugs to present best practice in

