1. Record Nr. UNINA9910817249603321

Autore	Ghosh Arun K.
Titolo	Structure-based design of drugs and other bioactive molecules : tools and strategies / / Arun K. Ghosh and Sandra Gemma
Pubbl/distr/stampa	Weinheim, Germany : , : Wiley-VCH, , 2014 ©2014
ISBN	3-527-66523-4 3-527-66521-8 3-527-66524-2
Descrizione fisica	1 online resource (476 p.)
Disciplina	615.190285
Soggetti	Drug development - Data processing Bioactive compounds - Analysis Biopolymers
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
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 Inhibitors2.4 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 Hydroxypyrone-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 Inhibitors2.8.5 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
3.7.1 Synthesis of -Aminoalkyl Boronic Acid Derivatives3.8 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
4.3.2 Development of -Lactone Natural Product-Based Proteasome Inhibitors4.3.3 Development of Epoxy Ketone-Derived Inhibitors; 4.3.4 Noncovalent Proteasome Inhibitors; 4.4 Synthesis of -Lactone Scaffold; 4.5 Synthesis of Epoxy Ketone Scaffold; 4.6 Conclusions; References; 5 Design of Cysteine Protease Inhibitors; 5.1 Introduction; 5.2 Development of Cysteine Protease Inhibitors with Michael Acceptors; 5.3 Design of Noncovalent Cysteine Protease Inhibitors; 5.4 Conclusions; References; 6 Design of Metalloprotease Inhibitors; 6.1 Introduction; 6.2 Design of Matrix Metalloprotease Inhibitors
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