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Titolo	Fragment-based approaches in drug discovery [[electronic resource] /] / edited by Wolfgang Jahnke and Daniel A. Erlanson
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Altri autori (Persone)	JahnkeWolfgang ErlansonDaniel A
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Nota di contenuto	Fragment-based Approaches in Drug Discovery; Contents; Preface; A Personal Foreword; List of Contributors; Part I: Concept and Theory; 1 The Concept of Fragment-based Drug Discovery; 1.1 Introduction; 1.2 Starting Small: Key Features of Fragment-based Ligand Design; 1.2.1 FBS Samples Higher Chemical Diversity; 1.2.2 FBS Leads to Higher Hit Rates; 1.2.3 FBS Leads to Higher Ligand Efficiency; 1.3 Historical Development; 1.4 Scope and Overview of this Book; References; 2 Multivalency in Ligand Design; 2.1 Introduction and Overview; 2.2 Definitions of Terms 2.3 Selection of Key Experimental Studies2.3.1 Trivalency in a Structurally Simple System; 2.3.2 Cooperativity (and the Role of Enthalpy) in the "Chelate Effect"; 2.3.3 Oligovalency in the Design of Inhibitors to Toxins; 2.3.4 Bivalency at Well Defined Surfaces (Self-assembled Monolayers, SAMs); 2.3.5 Polyvalency at Surfaces of Viruses, Bacteria, and SAMs; 2.4 Theoretical Considerations in Multivalency; 2.4.1 Survey of Thermodynamics; 2.4.2 Additivity and Multivalency;

2.4.3 Avidity and Effective Concentration (C(eff)); 2.4.4 Cooperativity is Distinct from Multivalency
2.4.5 Conformational Entropy of the Linker between Ligands2.4.6 Enthalpy/Entropy Compensation Reduces the Benefit of Multivalency; 2.5 Representative Experimental Studies; 2.5.1 Experimental Techniques Used to Examine Multivalent Systems; 2.5.1.1 Isothermal Titration Calorimetry; 2.5.1.2 Surface Plasmon Resonance Spectroscopy; 2.5.1.3 Surface Assays Using Purified Components (Cell-free Assays); 2.5.1.4 Cell-based Surface Assays; 2.5.2 Examination of Experimental Studies in the Context of Theory; 2.5.2.1 Trivalency in Structurally Simple Systems
2.5.2.2 Cooperativity (and the Role of Enthalpy) in the "Chelate Effect"
2.5.2.3 Oligovalency in the Design of Inhibitors of Toxins; 2.5.2.4 Bivalency in Solution and at Well Defined Surfaces (SAMs); 2.5.2.5 Polyvalency at Surfaces (Viruses, Bacteria, and SAMs); 2.6 Design Rules for Multivalent Ligands; 2.6.1 When Will Multivalency Be a Successful Strategy to Design Tight-binding Ligands?; 2.6.2 Choice of Scaffold for Multivalent Ligands; 2.6.2.1 Scaffolds for Oligovalent Ligands; 2.6.2.2 Scaffolds for Polyvalent Ligands; 2.6.3 Choice of Linker for Multivalent Ligands
2.6.3.1 Rigid Linkers Represent a Simple Approach to Optimize Affinity2.6.3.2 Flexible Linkers Represent an Alternative Approach to Rigid Linkers to Optimize Affinity; 2.6.4 Strategy for the Synthesis of Multivalent Ligands; 2.6.4.1 Polyvalent Ligands: Polymerization of Ligand Monomers; 2.6.4.2 Polyvalent Ligands: Functionalization with Ligands after Polymerization; 2.7 Extensions of Multivalency to Lead Discovery; 2.7.1 Hetero-oligovalency Is a Broadly Applicable Concept in Ligand Design; 2.7.2 Dendrimers Present Opportunities for Multivalent Presentation of Ligands
2.7.3 Bivalency in the Immune System

Sommario/riassunto

This first systematic summary of the impact of fragment-based approaches on the drug development process provides essential information that was previously unavailable. Adopting a practice-oriented approach, this represents a book by professionals for professionals, tailor-made for drug developers in the pharma and biotech sector who need to keep up-to-date on the latest technologies and strategies in pharmaceutical ligand design. The book is clearly divided into three sections on ligand design, spectroscopic techniques, and screening and drug discovery, backed by numerous case studies.

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