

Libros

Books

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El área de las simulaciones moleculares computacionales ha tomado mucha fuerza en los últimos años, sobre todo en el año 2013, cuando se otorgó el premio nobel de química a Michael Levitt, Martin Karplus y Arieh Warshel, quienes llevaron los experimentos químicos al ambiente virtual de las computadoras. Hoy en día, los avances tecnológicos permiten el uso de computadoras para asistir y ayudar a las personas en su quehacer diario, y la Química Farmacéutica no es la excepción. Aunque alguno de los libros presentado en esta sección contiene temas relacionados con todas las etapas del diseño de Fármacos, se presentan títulos que pueden interesar al lector para sumergirse en el área del diseño de fármacos asistido por computadora. Estos métodos en la actualidad, resultan sumamente atractivos pues en general son de bajo costo y pueden ser sumamente rápidos comparados con los métodos experimentales. En pocas palabras, se espera esta reseña proporcione al lector una visión general de las temáticas involucradas y los métodos computacionales utilizados en el diseño de nuevas moléculas con uso terapéutico.

The Practice of Medicinal Chemistry

Camille Georges Wermuth

Prestwick Chemical Inc.

3rd edition, 2008

942 pages

ISBN-13: 978-0123741943

De forma sumamente completa, este libro ofrece una perspectiva general en materia de diseño, desarrollo, síntesis, metabolismo y nomenclatura de fármacos, abordando aspectos de fármaco-economía. Incluye además, una serie de consideraciones en materia de formulaciones farmacéuticas referente a problemas que se pueden presentar ante la presencia de diferentes grupos funcionales en los fármacos. Pero no solo eso, otorga una relación entre los aspectos fisiológicos que son determinantes en las propiedades farmacocinéticas de los fármacos y su acción terapéutica. En resumen, es un compendio muy completo en materia de Química Farmacéutica elemental para todo profesional dedicado al diseño de fármacos, o que se interese en esta rama de las ciencias de la salud.

Part I: General Aspects of Medicinal Chemistry

1. A History of Drug Discovery
2. Medicinal Chemistry: Definitions and Objectives, Drug Activity Phases, Drug Classification Systems
3. Measurement and Expression of Drug Effects
4. Molecular Drug Targets
5. Drug Targets, Target Identification, Validation and Screening

Part II: Lead Compound Discovery Strategies

6. Strategies in the Search for New Lead Compounds or Original Working Hypotheses
7. High-Throughput Screening and Drug Discovery
8. Natural Products as Pharmaceuticals and Sources for Lead Structures
9. Biology Oriented Synthesis and Diversity Oriented Synthesis in Compound Collection Development
10. In Silico Screening: Hit Finding from Database Mining
11. Fragment-Based Drug Discovery
12. Lead-Likeness and Drug-Likeness
13. Web Alert: Using the Internet for Medicinal Chemistry

Part III: Primary Exploration of Structure–Activity Relationships

14. Molecular Variations in Homologous Series: Vinylogues and Benzologues
15. Molecular Variations Based on Isosteric Replacements
16. Ring Transformations
17. Conformational Restriction and/or Steric Hindrance in Medicinal Chemistry
18. Homo and Heterodimer Ligands the Twin Drug Approach
19. Application Strategies for the Primary Structure–Activity Relationship Exploration

Part IV: Substituents and Functions: Qualitative and Quantitative Aspects of Structure–Activity Relationships

20. Substituent Groups
21. The Role of Functional Groups in Drug–Receptor Interactions
22. Compound Properties and Drug Quality
23. Quantitative Approaches to Structure–Activity Relationships

Part V: Spatial Organization, Receptor Mapping and Molecular Modeling

24. Overview: The Search for Biologically Useful Chemical Space
25. Pharmacological Space
26. Optical Isomerism in Drugs
27. Multi-Target Drugs: Strategies and Challenges for Medicinal Chemists
28. Pharmacophore Identification and Pseudo-Receptor Modeling
29. 3D Quantitative Structure–Property Relationships
30. Protein Crystallography and Drug Discovery

Part VI: Chemical Modifications Influencing the Pharmacokinetic Properties

32. Biotransformation Reactions and their Enzymes
33. Biotransformations Leading to Toxic Metabolites: Chemical Aspects
34. Drug Transport Mechanisms and their Impact on the Disposition and Effects of Drugs
35. Strategies for Enhancing Oral Bioavailability and Brain Penetration
36. Designing Prodrugs and Bioprecursors

Part VII: Pharmaceutical and Chemical Means to Solubility and Formulation Problems

37. Preparation of Water-Soluble Compounds through Salt Formation
38. Preparation of Water-Soluble Compounds by Covalent Attachment of Solubilizing Moieties

39. Drug Solubilization with Organic Solvents, or Using Micellar Solutions or Other Colloidal Dispersed Systems
40. Improvement of Drug Properties by Cyclodextrins
41. Chemical and Physicochemical Approaches to Solve Formulation Problems

Part VIII: Development of New Drugs: Legal and Economic Aspects

42. Discover a Drug Substance, Formulate and Develop It to a Product
43. Drug Nomenclature
44. Legal Aspects of Product Protection: What a Medicinal Chemist Should Know about Patent Protection
45. The Consumption and Production of Pharmaceuticals

Structural Bioinformatics

Jenny Gu, Philip E. Bourne

Wiley-Blackwell

2nd Edition, 2009

1096 pages

ISBN: 978-0-470-18105-8

Actualmente las aplicación y uso de herramientas computacionales empleadas en el área biológica han sido ampliamente aceptadas, ya que ofrecen grandes ventajas a la hora de profundizar en los procesos bioquímicos a nivel molecular y a acelerar el descubrimiento y desarrollo de fármacos. Es por ello que se presenta este excelente libro que es un recurso valioso para una amplia gama de lectores en la bioinformática y campos de biología avanzada. Dentro de su contenido se muestran teorías, algoritmos, los recursos y las herramientas utilizadas en el análisis, predicción y fundamentos teóricos de ADN, ARN y proteínas. En un libro que debe formar parte de su acervo cultural y de su biblioteca personal.

Section I DATA COLLECTION, ANALYSIS, AND VISUALIZATION

- 1 DEFINING BIOINFORMATICS AND STRUCTURAL BIOINFORMATICS
- 2 FUNDAMENTALS OF PROTEIN STRUCTURE
- 3 FUNDAMENTALS OF DNA AND RNA STRUCTURE
- 4 COMPUTATIONAL ASPECTS OF HIGH-THROUGHPUT CRYSTALLOGRAPHIC MACROMOLECULAR STRUCTURE DETERMINATION
- 5 MACROMOLECULAR STRUCTURE DETERMINATION BY NMR SPECTROSCOPY
- 6 ELECTRON MICROSCOPY IN THE CONTEXT OF STRUCTURAL SYSTEMS BIOLOGY

7 STUDY OF PROTEIN THREE-DIMENSIONAL STRUCTURE AND DYNAMICS USING PEPTIDE AMIDE HYDROGEN/DEUTERIUM EXCHANGE MASS SPECTROMETRY (DXMS) AND CHEMICAL CROSS-LINKING WITH MASS SPECTROMETRY TO CONSTRAIN MOLECULAR MODELING

8 SEARCH AND SAMPLING IN STRUCTURAL BIOINFORMATICS

9 MOLECULAR VISUALIZATION

Section II DATA REPRESENTATION AND DATABASES

10 THE PDB FORMAT, mmCIF FORMATS, AND OTHER DATA FORMATS

11 THE WORLDWIDE PROTEIN DATA BANK

12 THE NUCLEIC ACID DATABASE

13 OTHER STRUCTURE-BASED DATABASES

Section III DATA INTEGRITY AND COMPARATIVE FEATURES

14 STRUCTURAL QUALITY ASSURANCE

15 THE IMPACT OF LOCAL ACCURACY IN PROTEIN AND RNA STRUCTURES: VALIDATION AS AN ACTIVE TOOL

16 STRUCTURE COMPARISON AND ALIGNMENT

17 PROTEIN STRUCTURE EVOLUTION AND THE SCOP DATABASE

18 THE CATH DOMAIN STRUCTURE DATABASE

Section IV STRUCTURAL AND FUNCTIONAL ASSIGNMENT

19 SECONDARY STRUCTURE ASSIGNMENT

20 IDENTIFYING STRUCTURAL DOMAINS IN PROTEINS

21 INFERRING PROTEIN FUNCTION FROM STRUCTURE

22 STRUCTURAL ANNOTATION OF GENOMES

23 EVOLUTION STUDIED USING PROTEIN STRUCTURE

Section V MACROMOLECULAR INTERACTIONS

24 ELECTROSTATIC INTERACTIONS

25 PREDICTION OF PROTEIN-NUCLEIC ACID INTERACTIONS

26 PREDICTION OF PROTEIN-PROTEIN INTERACTIONS FROM EVOLUTIONARY INFORMATION

27 DOCKING METHODS, LIGAND DESIGN, AND VALIDATING DATA SETS IN THE STRUCTURAL GENOMICS ERA

Section VII THERAPEUTIC DISCOVERY

34 STRUCTURAL BIOINFORMATICS IN DRUG DISCOVERY

35 B-CELL EPITOPE PREDICTION

Section VIII FUTURE CHALLENGES

36 METHODS TO CLASSIFY AND PREDICT THE STRUCTURE OF MEMBRANE PROTEINS

37 PROTEIN MOTION: SIMULATION

38 THE SIGNIFICANCE AND IMPACTS OF PROTEIN DISORDER AND CONFORMATIONAL VARIANTS

39 PROTEIN DESIGNABILITY AND ENGINEERING

40 STRUCTURAL GENOMICS OF PROTEIN SUPERFAMILIES

Molecular Modeling Basic Principles and Applications

Holtje H, Sippl W, Rognan D, Folkers G

Wiley

2nd edition, 2003

228 pages

ISBN 3-527-30589-0

La importancia de este libro radica en la simplicidad en que está escrito; sin que esta cualidad, demerite de algún modo lo fundamental de su contenido. Este libro, escrito por renombrados expertos en modelado molecular, explica los conceptos básicos de este tema de una manera avezada, y al mismo tiempo, fácilmente comprensible, haciendo de este libro, un texto ideal tanto para principiantes como para investigadores y estudiantes de posgrado que estudian Modelado Molecular, Química Computacional y Bioquímica. Un libro de primera línea que debe leer toda persona interesada en temas de Modelado Molecular.

Introduction

Small Molecules

- Generation of 3D-Coordinates
- Computational Tools for Geometry Optimization
- Conformational Analysis
- Determination of Molecular Interaction Potentials
- Pharmacophore Identification
- 3D QSAR Methods

A Case Study for Small Molecule Modeling: Dopamine D3 Receptor Antagonists

- Building a Pharmacophore Model
- 3D QSAR Analysis

Introduction to Comparative Protein Modeling

- Where and How to get Information on Proteins
- Terminology and Principles of Protein Structure
- Comparative Protein Modeling
- Optimization Procedures
- Model Refinement
- Molecular Dynamics
- Validation of Protein Models
- Properties of Proteins

Virtual Screening and Docking

- Preparation of the Partners
- Docking Algorithms
- Scoring Functions
- Postfiltering Virtual Screening Results
- Comparison of Different Docking and Scoring Methods
- Examples of successful Virtual Screening Studies

Scope and Limits of Molecular Docking

- Docking in the Polar Active Site that Contains Water Molecules – Viral Thymidine Kinases
- Learning from Results

Example for the Modeling of Protein-Ligand Complexes: Antigen Presentation by MHC Class I

- The Biochemical and Pharmacological Description of the Problem
- Molecular Modeling of the Antigen Complex Between a Viral Peptide and a Class I MHC

Glycoprotein

- Molecular Dynamics Studies of MHC-Peptide Complexes
- Analysis of models that Emerged from Molecular Dynamics
- SAR of the antigenic peptides from Molecular Dynamics
- How far does the Model Hold?
- The T-Cell Receptor comes in
- Some Concluding Remarks