

Ariel Fernández

Transformative Concepts for Drug Design: Target Wrapping

 Springer

Transformative Concepts For Drug Design Target Wrapping

Ariel Fernandez



Transformative Concepts For Drug Design Target Wrapping:

Transformative Concepts for Drug Design: Target Wrapping Ariel Fernandez, 2010-04-28 In spite of the enticing promises of the post genomic era the pharmaceutical world is in a state of disarray Drug discovery seems now riskier and more uncertain than ever Thus projects get routinely terminated in mid stage clinical trials new targets are getting harder to find and successful therapeutic agents are often recalled as unanticipated side effects are discovered Exploiting the huge output of genomic studies to make safer drugs has proven to be much more difficult than anticipated More than ever the lead in the pharmaceutical industry depends on the ability to harness innovative research and this type of innovation can only come from one source fundamental knowledge This book squarely addresses this crucial problem since it introduces fundamental discoveries in basic biomolecular research that hold potential to broaden the technological base of the pharmaceutical industry The book takes a fresh and fundamental look at the problem of how to design an effective drug with controlled specificity Since the novel transformative concepts are unfamiliar to most practitioners the first part of this book explains matters very carefully starting from a fairly elementary physico chemical level The second part of the book is devoted to practical applications aiming at nothing less than a paradigm shift in drug design This book is addressed to scientists working at the cutting edge of research in the pharmaceutical industry but the material is at the same time accessible to senior undergraduates or graduate students interested in drug discovery and molecular design [Physics at the Biomolecular Interface](#) Ariel Fernández, 2016-05-11 This book focuses primarily on the role of interfacial forces in understanding biological phenomena at the molecular scale By providing a suitable statistical mechanical apparatus to handle the biomolecular interface the book becomes uniquely positioned to address core problems in molecular biophysics It highlights the importance of interfacial tension in delineating a solution to the protein folding problem in unravelling the physico chemical basis of enzyme catalysis and protein associations and in rationally designing molecular targeted therapies Thus grounded in fundamental science the book develops a powerful technological platform for drug discovery while it is set to inspire scientists at any level in their careers determined to address the major challenges in molecular biophysics The acknowledgment of how exquisitely the structure and dynamics of proteins and their aqueous environment are related attests to the overdue recognition that biomolecular phenomena cannot be effectively understood without dealing with interfacial behaviour There is an urge to grasp how biologically relevant behaviour is shaped by the structuring of biomolecular interfaces and how interfacial tension affects the molecular events that take place in the cell This book squarely addresses these needs from a physicist perspective The book may serve as a monograph for practitioners and alternatively as an advanced textbook Fruitful reading requires a background in physical chemistry and some basics in biophysics The selected problems at the end of the chapters and the progression in conceptual difficulty make it a suitable textbook for a graduate level course or an elective course for seniors majoring in chemistry physics biomedical engineering or related disciplines

Biomolecular Interfaces Ariel Fernández Stigliano, 2015-04-20 The book focuses on the aqueous interface of biomolecules a vital yet overlooked area of biophysical research Most biological phenomena cannot be fully understood at the molecular level without considering interfacial behavior The author presents conceptual advances in molecular biophysics that herald the advent of a new discipline epiststructural biology centered on the interactions of water and bio molecular structures across the interface The author introduces powerful theoretical and computational resources in order to address fundamental topics such as protein folding the physico chemical basis of enzyme catalysis and protein associations On the basis of this information a multi disciplinary approach is used to engineer therapeutic drugs and to allow substantive advances in targeted molecular medicine This book will be of interest to scientists students and practitioners in the fields of chemistry biophysics and biomedical engineering

Computational and Visualization Techniques for Structural Bioinformatics Using Chimera Forbes J. Burkowski, 2014-07-29 A Step by Step Guide to Describing Biomolecular Structure Computational and Visualization Techniques for Structural Bioinformatics Using Chimera shows how to perform computations with Python scripts in the Chimera environment It focuses on the three core areas needed to study structural bioinformatics biochemistry mathematics and computation Und

Artificial Intelligence Platform For Molecular Targeted Therapy: A Translational Science Approach Ariel Fernandez, 2021-03-12 In the era of big biomedical data there are many ways in which artificial intelligence AI is likely to broaden the technological base of the pharmaceutical industry Cheminformatic applications of AI involving the parsing of chemical space are already being implemented to infer compound properties and activity By contrast dynamic aspects of the design of drug target interfaces have received little attention due to the inherent difficulties in dealing with physical phenomena that often do not conform to simplifying views This book focuses precisely on dynamic drug target interfaces and argues that the true game change in pharmaceutical discovery will come as AI is enabled to solve core problems in molecular biophysics that are intimately related to rational drug design and drug discovery Here are a few examples to convey the flavor of our quest How do we therapeutically impair a dysfunctional protein with unknown structure or regulation but known to be a culprit of disease In regards to SARS CoV 2 what is the structural impact of a dominant mutation how does the structure change translate into a fitness advantage what new therapeutic opportunity arises How do we extend molecular dynamics simulations to realistic timescales to capture the rare events associated with drug targeting in vivo How do we control specificity in drug design to selectively remove side effects This is the type of problems directly related to the understanding of drug target interfaces that the book squarely addresses by leveraging a comprehensive AI empowered approach

Topological Dynamics in Metamodel Discovery with Artificial Intelligence Ariel Fernández, 2022-12-21 The leveraging of artificial intelligence AI for model discovery in dynamical systems is cross fertilizing and revolutionizing both disciplines heralding a new era of data driven science This book is placed at the forefront of this endeavor taking model discovery to the next level Dealing with artificial intelligence

this book delineates AI's role in model discovery for dynamical systems. With the implementation of topological methods to construct metamodels, it engages with levels of complexity and multiscale hierarchies hitherto considered off limits for data science. Key Features: Introduces new and advanced methods of model discovery for time series data using artificial intelligence; Implements topological approaches to distill machine intuitive models from complex dynamics data; Introduces a new paradigm for a parsimonious model of a dynamical system without resorting to differential equations; Heralds a new era in data driven science and engineering based on the operational concept of computational intuition. Intended for graduate students, researchers and practitioners interested in dynamical systems empowered by AI or machine learning and in their biological engineering and biomedical applications, this book will represent a significant educational resource for people engaged in AI related cross disciplinary projects. *Biopolymers for Medical Applications* Juan M. Ruso, Paula V. Messina, 2017-02-17

This book presents an experimental and computational account of the applications of biopolymers in the field of medicine. Biopolymers are macromolecules produced by living systems such as proteins, polypeptides, nucleic acids and polysaccharides. Their advantages over polymers produced using synthetic chemistry include diversity, abundance, relatively low cost and sustainability. This book explains techniques for the production of different biodevices such as scaffolds, hydrogels, functional nanoparticles, microcapsules and nanocapsules. Furthermore, developments in nanodrug delivery, gene therapy and tissue engineering are described. **Membrane Hydration** E. Anibal Disalvo, 2015-10-05 This book is about the importance of water in determining the structure, stability and responsive behavior of biological membranes. Water confers to lipid membranes unique features in terms of surface and mechanical properties. The analysis of the hydration forces, plasticiser effects, controlled hydration, formation of microdomains of confined water suggests that water is an active constituent in a water lipid system. The chapters describe water organization at the lipid membrane water interphase, the water penetration, the long range water structure in the presence of lipid membranes by means of X ray and neutron scattering, general polarization, fluorescent probes, ATR FTIR and near infrared spectroscopies, piezo electric methods, computer simulation and surface thermodynamics. Permeation, percolation, osmotic stress, polarization, protrusion, sorption, hydrophobicity, density fluctuations are treated in detail in self assembled bilayers. Studies in lipid monolayers show the correlation of surface pressure with water activity and its role in peptide and enzyme interactions. The book concludes with a discussion on anhydrobiosis and the effect of water replacement in microdomains and its consequence for cell function. New definitions of lipid water interphases consider water not only as a structural making solvent but as a mediator in signalling, metabolic activity, modulating protein insertion and enzymatic activity, triggering oscillatory reactions and functioning of membrane bound receptors. Since these effects occur at the molecular level, membrane hydration appears fundamental to understand the behavior of nano systems and confined environments mimicking biological systems. These insights in structural, thermodynamical and mechanical water properties give a base for new paradigms in membrane structure and

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Table of Contents Transformative Concepts For Drug Design Target Wrapping

1. Understanding the eBook Transformative Concepts For Drug Design Target Wrapping
 - The Rise of Digital Reading Transformative Concepts For Drug Design Target Wrapping
 - Advantages of eBooks Over Traditional Books
2. Identifying Transformative Concepts For Drug Design Target Wrapping
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Transformative Concepts For Drug Design Target Wrapping
 - User-Friendly Interface
4. Exploring eBook Recommendations from Transformative Concepts For Drug Design Target Wrapping
 - Personalized Recommendations
 - Transformative Concepts For Drug Design Target Wrapping User Reviews and Ratings

- Transformative Concepts For Drug Design Target Wrapping and Bestseller Lists
- 5. Accessing Transformative Concepts For Drug Design Target Wrapping Free and Paid eBooks
 - Transformative Concepts For Drug Design Target Wrapping Public Domain eBooks
 - Transformative Concepts For Drug Design Target Wrapping eBook Subscription Services
 - Transformative Concepts For Drug Design Target Wrapping Budget-Friendly Options
- 6. Navigating Transformative Concepts For Drug Design Target Wrapping eBook Formats
 - ePub, PDF, MOBI, and More
 - Transformative Concepts For Drug Design Target Wrapping Compatibility with Devices
 - Transformative Concepts For Drug Design Target Wrapping Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Transformative Concepts For Drug Design Target Wrapping
 - Highlighting and Note-Taking Transformative Concepts For Drug Design Target Wrapping
 - Interactive Elements Transformative Concepts For Drug Design Target Wrapping
- 8. Staying Engaged with Transformative Concepts For Drug Design Target Wrapping
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Transformative Concepts For Drug Design Target Wrapping
- 9. Balancing eBooks and Physical Books Transformative Concepts For Drug Design Target Wrapping
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Transformative Concepts For Drug Design Target Wrapping
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Transformative Concepts For Drug Design Target Wrapping
 - Setting Reading Goals Transformative Concepts For Drug Design Target Wrapping
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Transformative Concepts For Drug Design Target Wrapping
 - Fact-Checking eBook Content of Transformative Concepts For Drug Design Target Wrapping
 - Distinguishing Credible Sources

13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
 - Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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