

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 epistuctural 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 function for

those interested in biophysics physical chemistry biology bio and nano medicine biochemistry biotechnology and nano sciences searching for biotechnological inputs in human health food industry plant growing and energy conversion

**Flying Magazine** ,1966-11      **Government Reports Announcements & Index** ,1990      **Transformative Concepts for Drug Design** Ariel Fernandez,2010 Introduces fundamental discoveries in basic biomolecular research that hold potential to broaden the technological base of the pharmaceutical industry This book takes a fresh and fundamental look at the problem of how to design an effective drug with controlled specificity      **Targeted Drug Delivery : Concepts and Design** Padma V. Devarajan,Sanyog Jain,2014-12-08 This authoritative volume explores the fundamental concepts and numerous applications of targeted delivery of drugs to the body This compilation has been divided into eight sections comprised of the basic principles of drug targeting disease and organ organelle based targeting passive and active targeting strategies and various advanced drug delivery tools such as functionalized lipidic polymeric and inorganic nanocarriers Together the twenty three chapters cover a wide range of topics in the field including tumor and hepatic targeting polymer drug conjugates nanoemulsion physical and biophysical characteristics of nanoparticles and in vivo imaging techniques among others The book also examines advanced characterization techniques regulatory hurdles and toxicity related issues that are key features for successful commercialization of targeted drug delivery system products Targeted Drug Delivery is a comprehensive reference guide for drug delivery researchers both beginners and those already working in the field      **Drug Targeting And Delivery** H.E. Junginger,1992-10-31 This is a review of the structure and function of biological membranes and other cellular barriers used in drug transport It discusses a range of concepts for drug delivery systems treating the routes of drugs with regard to their characteristics function structure uptake mechanism and effect The book also explores the interface between pharmaceutical technology and physiological principles in drug design a field of increased importance to industry      *Drug Target Selection and Validation* Marcus T. Scotti,Carolina L. Bellera,2023-05-19 The first book in the newly created book series Computer Aided Drug Discovery and Design focuses on the computational aspects of early drug discovery drug target identification and validation It revises current classical paradigms in target and phenotypic based drug design with still ingrained approximations and concepts and discusses the research in the new network approach concept that include kinetic selectivity and metabolic analysis Many often overlooked approximations and concepts in drug discovery are fully covered Drug Target Selection and Validation includes both introductory sections and research based sections to be of use to both students and research scientists in drug discovery design kinetics and metabolic analysis Pharmaceutical scientists pharmaceutics drug developers pharmacologists biomedical researchers in computer science medicinal chemists and precision medicine developers benefit from the information provided The book concludes with a chapter on chemical and structural databases      **Peptide-Based Drug Design** Laszlo Otvos,2008-10-09 Due to their high specificity and low toxicity profile peptides have once again become central to the development of new drugs In Peptide Based Drug Design Methods

and Protocols expert researchers provide a handbook which offers a selection of research and production tools suitable for transforming a promising protein fragment or stand alone native peptide into a pharmaceutically acceptable composition The volume delves into contemporary cutting edge subjects such as hit isolation and target validation computer aided design sequence modifications to satisfy pharmacologists in vivo stability and imaging and the actual production of difficult sequences Written in the highly successful Methods in Molecular Biology™ series format chapters include readily reproducible step by step laboratory protocols lists of materials and the Notes section which highlights tips on troubleshooting and avoiding known pitfalls Comprehensive and up to date Peptide Based Drug Design Methods and Protocols shows its subject to be an independent science on the rise and provides scientists with a clear concise guide for continuing this vital research

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