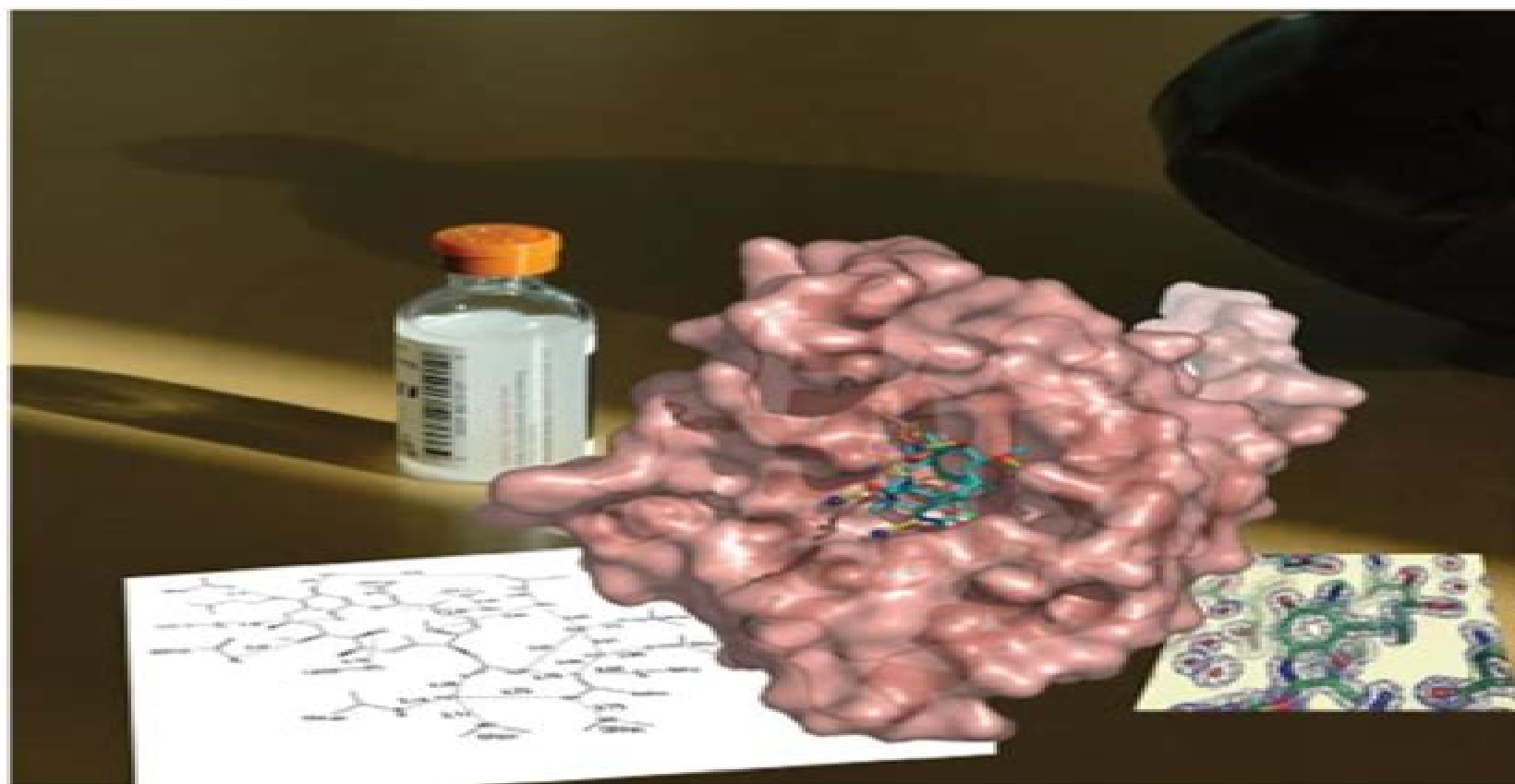


RSC Biomolecular Sciences

Edited by Robert M Stroud and Janet Finer-Moore

Computational and Structural Approaches to Drug Discovery

Ligand Protein Interactions



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Computational And Structural Approaches To Drug Discovery Ligand Protein Interactions Rsc Biomolecular Sciences

Keith R Fox, Tom Brown



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Computational and Structural Approaches to Drug Discovery Robert Stroud, Janet Finer-Moore, 2007-10-31

Computational methods impact all aspects of modern drug discovery and most notably these methods move rapidly from academic exercises to becoming drugs in clinical trials This insightful book represents the experience and understanding of the global experts in the field and spotlights both the structural and medicinal chemistry aspects of drug design The need to encode the factors that determine adsorption distribution metabolism excretion and toxicology are explored as they remain the critical issues in this area of research This indispensable resource provides the reader with A rich understanding of modern approaches to docking A comparison and critical evaluation of state of the art methods Details on harnessing computational methods for both analysis and prediction An insight into prediction potencies and protocols for unbiased evaluations of docking and scoring algorithms Critical reviews of current fragment based methods with perceptive applications to kinases Addressing a wide range of uses of protein structures for drug discovery the Editors have created an essential reference for professionals in the pharmaceutical industry and moreover an indispensable core text for all graduate level courses covering molecular interactions and drug discovery

Computational and Structural Approaches to Drug Discovery Robert M. Stroud, Janet Finer-Moore, 2008

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in Structure Based Drug Design Jeanne A Hardy 18 The Impact of Protein Kinase Structures on Drug Discovery Chao Zhang and Sung Hou Kim Biophysical Approaches Determining Ligand Binding to Biomolecular Targets Alberto Podjarny, Annick P Dejaegere, Bruno Kieffer, 2011-04-01 The binding of small ligands to biological molecules is central to most aspects of biological function The past twenty years has seen the development of an increasing armoury of biophysical methods that not only detect such binding but also provide varying degrees of information about the kinetics thermodynamics and structural aspects of the process These methods have received increasing attention with the growth in more rational approaches to drug discovery and design This book reviews the latest advances in the application of biophysics to the study of ligand binding It provides a complete overview of current techniques to identify ligands characterise their binding sites and understand their binding mechanisms Particular emphasis is given to the combined use of different techniques and their relative strengths and weaknesses Consistency in the way each technique is described makes it easy for readers to select the most suitable protocol for their research The introduction explains why some techniques are more suitable than others and emphasizes the possible synergies between them The following chapters all written by a specialist in the particular technique focus on each method individually The book finishes by describing how several complimentary techniques can be used together for maximum effectiveness This book is suitable for biomolecular scientists at graduate or post doctoral level in academia and industry Biologists and chemists will also find it a useful introduction to the techniques available

Innovations in Biomolecular Modeling and Simulations Tamar Schlick, 2012 The chemical and biological sciences face unprecedented opportunities in the 21st century A confluence of factors from parallel universes advances in experimental techniques in biomolecular structure determination progress in theoretical modeling and simulation for large biological systems and breakthroughs in computer technology has opened new avenues of opportunity as never before Now experimental data can be interpreted and further analysed by modeling and predictions from any approach can be tested and advanced through companion methodologies and technologies This two volume set describes innovations in biomolecular modeling and simulation in both the algorithmic and application fronts With contributions from experts in the field the books describe progress and innovation in areas including simulation algorithms for dynamics and enhanced configurational sampling force field development implicit solvation models coarse grained models quantum mechanical simulations protein folding DNA polymerase mechanisms nucleic acid complexes and simulations RNA structure analysis and design and other important topics in structural biology modeling The books are aimed at graduate students and experts in structural biology and chemistry and the emphasis is on reporting innovative new approaches rather than providing comprehensive reviews on each subject *Natural Product Chemistry for Drug Discovery* Antony D. Buss, Mark S. Butler, 2010 This text provides a comprehensive summary of where natural product chemistry is today in drug discovery It covers emerging technologies and case studies and is a source of up to date information on the topical subject of natural products **Structural Virology**

Mavis Agbandje-McKenna, Robert McKenna, 2010-11-11 Over the last ten years much effort has been devoted to improving the biophysical techniques used in the study of viruses This has resulted in the visualization of these large macromolecular assemblages at atomic level thus providing the platform for functional interpretation and therapeutic design Structural Virology covers a wide range of topics and is split into three sections The first discusses the vast biophysical methodologies used in structural virology including sample production and purification confocal microscopy mass spectrometry negative stain and cryo electron microscopy X ray crystallography and nuclear magnetic resonance spectroscopy The second discusses the role of virus capsid protein structures in determining the functional roles required for receptor recognition cellular entry capsid assembly genome packaging and mechanisms of host immune system evasion The last section discusses therapeutic strategies based on virus protein structures including the design of antiviral drugs and the development of viral capsids as vehicles for foreign gene delivery Each topic covered will begin with a review of the current literature followed by a more detailed discussion of experimental procedures a step in the viral life cycle or strategies for therapeutic development With contributions from experts in the field of structural biology and virology this exceptional monograph will appeal to biomedical scientists involved in basic and or applied research on viruses It also provides up to date reference material for students entering the field of structural virology as well as scientists already familiar with the area Nucleic Acid-metal Ion Interactions

Nicholas V. Hud, 2009 Provides a perspective on nucleic acid metal ion interactions with an emphasis on experimental biophysical studies which will prove indispensable to biophysicists and molecular biologists **Ribozymes and RNA Catalysis** David Malcolm James Lilley, Fritz Eckstein (Professor.), 2008 Takes the reader through the origins of catalysis in RNA and necessarily includes significant discussion of structure and folding The main focus of the book concerns chemical mechanism with extensive comment on how despite the importance of RNA catalysis in the cell its origins are still poorly understood and often controversial The reader is given an outline of the important role of RNA catalysis in many aspects of cell function including RNA processing and translation Recent Developments in Biomolecular NMR

Marius Clore, Jennifer Potts, 2012-08-21 NMR spectroscopy is widely used in biomolecular science particularly for structure determination of proteins nucleic acids and carbohydrates Much of the innovation within NMR spectroscopy has been within the field of protein NMR spectroscopy an important technique in structural biology Filling a gap in the literature this book draws together experts in the field to discuss the real advances in NMR methods that have occurred or have an impact on the biomolecular field in the last few years The coverage includes recent developments in using NMR for determination of protein structures membrane proteins the dynamics of RNA and advances in NMR in drug discovery Edited by leading biological NMR spectroscopists the book is essential reference for researchers in industry and academia interested in or joining this bioanalytical field DNA Conjugates and Sensors Keith R Fox, Tom Brown, 2012-11-30 Applications of nucleic acids have developed recently to provide solutions for biosensors diagnostic tools and as platforms for the assembly of

complex structures These developments have been possible as their base sequence can be used to assemble precise structures following simple and predictable rules Self assembled DNA can then be amplified using polymerase chain reaction PCR and this ultimately enables the preparation of synthetic nucleic acids Their use as molecular tools or DNA conjugates has recently been enhanced by the addition of other groups including enzymes fluorophores and small molecules Written by leaders in the field this volume describes the preparation and application of these DNA conjugates Several have been used as sensors aptamers riboswitches and nanostructures based on the ability of nucleic acids to adopt specific structures in the presence of ligands whilst others link reporter groups such as proteins or fluorophores to RNA or DNA for detection single molecule studies and increasing the sensitivity of PCR The book is relevant to researchers in areas related to analytical chemistry chemical biology medicinal chemistry molecular pharmacology and structural and molecular biology

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