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There are two computational techniques that can aid in understanding and optimizing drug–target binding kinetics – molecular dynamics (MD) and machine learning (ML). For both ligand–protein structures ...

Improving Drug–Receptor Interactions To Make Medicines Work Better

The Organisation for Economic Co-operation and Development (OECD) has approved the first overall testing strategy to predict skin allergic reactions without using animals.

Non-animal test for skin sensitisation gets OECD approval

The central purpose of this book is to illustrate the premise that examination of the kinetics of biological processes can ... Topics covered range from co-operativity in protein binding, through ...

Biological Kinetics

The Multidisciplinary Molecular Interaction Core (MMIC) provides use of a Biacore T200 biosensor that is capable of determining the binding kinetics, specificities, and thermodynamics of biomolecular ...

Multidisciplinary Molecular Interaction Core (MMIC)

We have instrumentation ideal for acquiring high quality kinetic, affinity and thermodynamic data for biomolecular interactions. Our facility enables you to achieve direct, label-free measurement of ...

Molecular Interactions

Binding of the substrate in an initial weak-binding ... We are using our sophisticated structural and kinetic methods to understand the molecular basis for these defects. Understanding the ...

Kenneth Johnson

To probe the role of zinc as an anti-SARS-CoV-2 agent at the structural and molecular level, researchers in India studied the binding kinetics and the inhibition mechanism of zinc with SARS-CoV-2 ...

Zinc inhibits SARS-CoV-2's main protease in vitro

(2011) "Substrate binding drives large-scale conformational changes in the Hsp90 molecular chaperone ... (2009) "Predicting repeat protein folding kinetics from an experimentally determined folding ...

Molecular and Cell Biology Program

Label-free detection can be performed in a single step while also enabling real-time monitoring and determination of the binding kinetics involved in the interaction ... suitable for reliable ...

Single-step label-free nanowell immunoassay accurately quantifies serum stress hormones within minutes

However, physicochemical differences arising from the binding of analog to the solid support confer kinetic differences that results in decreased analog affinity for endogenous binding proteins ...

Free Thyroxine (FT4) and Free Triiodothyronine (FT3) Estimate Tests

In addition, the idea that we are all large assemblies of tiny molecular machines was fascinating to me ... We were able to show that phosphorylation of the GS region transforms it from a binding site ...

At Work: Immunologist Morgan Huse

To probe the role of zinc as an anti-SARS-CoV-2 agent at the structural and molecular level, researchers in India studied the binding kinetics and the inhibition mechanism of zinc with SARS-CoV-2 ...

Zinc News and Research

Ongoing advances and breakthroughs in synthesis and experimental characterization techniques yield increasing detailed molecular-level information ... Peslherbe, “Transitioning to a Hydrogen Economy: ...

Gilles Peslherbe, PhD

in contrast to the Hedgehog binding site—which is shielded from the membrane and exposed to the aqueous environment of the ER—large cavities in DGAT1 and ACAT1 are directly exposed to the luminal ...

Substrate and product complexes reveal mechanisms of Hedgehog acylation by HHAT

Department of Molecular Biology, Princeton University ... protein 16 (IFI16), which moves to the nuclear periphery and forms oligomeric assemblies upon binding to vDNA (3–6). This host protein–vDNA ...

Systematic profiling of protein complex dynamics reveals DNA-PK phosphorylation of IFI16 en route to herpesvirus immunity

Techniques vary with the particular project, and can entail molecular biology, organic synthesis, protein crystallography and NMR spectroscopy as well as protein purification, enzyme kinetics and ...

This handbook offers a practical guide to the principles of quantitative analysis in biological experiments. The material is primarily aimed at working molecular biologists, but the scope and clarity of presentation make it equally suitable as an introduction for students. Topics covered range from the basics â€” such as measuring the concentrations of macromolecules â€” through considerations of binding constants and the kinetics of molecular interactions. The book ends with a thorough consideration of data analysis.

This practical reference for medicinal and pharmaceutical chemists combines the theoretical background with modern methods as well as applications from recent lead finding and optimization projects. Divided into two parts on the thermodynamics and kinetics of drug-receptor interaction, the text provides the conceptual and methodological basis for characterizing binding mechanisms for drugs and other bioactive molecules. It covers all currently used methods, from experimental approaches, such as ITC or SPR, right up to the latest computational methods. Case studies of real-life lead or drug development projects are also included so readers can apply the methods learned to their own projects. Finally, the benefits of a thorough binding mode analysis for any drug development project are summarized in an outlook chapter written by the editors.

Progressively builds a deep understanding of macromolecular behavior Based on each of the authors' roughly forty years of biophysics research and teaching experience, this text instills readers with a deep understanding of the biophysics of macromolecules. It sets a solid foundation in the basics by beginning with core physical concepts such as thermodynamics, quantum chemical models, molecular structure and interactions, and water and the hydrophobic effect. Next, the book examines statistical mechanics, protein-ligand binding, and conformational stability. Finally, the authors address kinetics and equilibria, exploring underlying theory, protein folding, and stochastic models. With its strong emphasis on molecular interactions, Equilibria and Kinetics of Biological Macromolecules offers new insights and perspectives on proteins and other macromolecules. The text features coverage of: Basic theory, applications, and new research findings Related topics in thermodynamics, quantum mechanics, statistical mechanics, and molecular simulations Principles and applications of molecular simulations in a dedicated chapter and interspersed throughout the text Macromolecular binding equilibria from the perspective of statistical mechanics Stochastic processes related to macromolecules Suggested readings at the end of each chapter include original research papers, reviews and monographs, enabling readers to explore individual topics in greater depth. At the end of the text, ten appendices offer refreshers on mathematical treatments, including probability, computational methods, Poisson equations, and defining molecular boundaries. With its classroom-tested pedagogical approach, Equilibria and Kinetics of Biological Macromolecules is recommended as a graduate-level textbook for biophysics courses and as a reference for researchers who want to strengthen their understanding of macromolecular behavior.

The application of biosensors is expanding in different areas. These are portable and convenient devices that permit the rapid, accurate, and reliable detection of analytes of interest present either in the atmosphere or in aqueous or in liquid phases. The detection of glucose levels in blood for the effective management of diabetes is one. Though different biosensors have been designed for an increasing number of applications, the kinetics of binding (and dissociation) of analytes by the receptors on the biosensor surfaces has not been given enough attention in the open literature. This is a very important area of investigation since it significantly impacts biosensor performance parameters such as stability, sensitivity, selectivity, response time, regenerability, etc. Binding and Dissociation Kinetics for Different Biosensor Applications Using Fractals addresses this critical need besides helping to correct or demonstrate the need to modify the present software available with commercial biosensors that determines the kinetics of analyte-receptor reactions on biosensor surfaces. * first book to provide detailed kinetic analysis of the binding and dissociation reactions that are occuring on the biosensor surface * addresses the area of analyte-receptor binding and dissociation kinetics occurring on biosensor surfaces * provides physical insights into reactions occuring on biosensor surfaces

"a gem of a textbook which manages to produce a genuinely fresh, concise yet comprehensive guide" –Mark Leake, University of York "destined to become a standard reference.... Not just a ‘how to’ handbook but also an accessible primer in the essentials of kinetic theory and practice." –Michael Geeves, University of Kent "covers the entire spectrum of approaches, from the traditional steady state methods to a thorough account of transient kinetics and rapid reaction techniques, and then on to the new single molecule techniques" –Stephen Halford, University of Bristol This illustrated treatment explains the methods used for measuring how much a reaction gets speeded up, as well as the framework for solving problems such as ligand binding and macromolecular folding, using the step-by-step approach of numerical integration. It is a thoroughly modern text, reflecting the recent ability to observe reactions at the single-molecule level, as well as advances in microfluidics which have given rise to femtoscale studies. Kinetics is more important now than ever, and this book is a vibrant and approachable entry for anyone who wants to understand mechanism using transient or single molecule kinetics without getting bogged down in advanced mathematics. Clive R. Bagshaw is Emeritus Professor at the University of Leicester, U.K., and Research Associate at the University of California at Santa Cruz, U.S.A.

The overall picture of molecular recognition covers the thermodynamic and kinetic properties of molecular systems. Regarding thermodynamics, binding affinity or free energy, which can be decomposed into enthalpy and entropy, determines the strength of binding. Binding kinetics, the association and dissociation rate constants, describe the rates for molecular binding and unbinding. In this thesis, I carried out various molecular mechanics modeling tools to understand binding thermodynamics and kinetics of host-guest systems and protein-ligand systems.

Innovative and forward-looking, this volume focuses on recent achievements in this rapidly progressing field and looks at future potential for development. The first part provides a basic understanding of the factors governing protein-ligand interactions, followed by a comparison of key experimental methods (calorimetry, surface plasmon resonance, NMR) used in generating interaction data. The second half of the book is devoted to insilico methods of modeling and predicting molecular recognition and binding, ranging from first principles-based to approximate ones. Here, as elsewhere in the book, emphasis is placed on novel approaches and recent improvements to established methods. The final part looks at unresolved challenges, and the strategies to address them. With the content relevant for all drug classes and therapeutic fields, this is an inspiring and often-consulted guide to the complexity of protein-ligand interaction modeling and analysis for both novices and experts.

Biochemical kinetics refers to the rate at which a reaction takes place. Kinetic mechanisms have played a major role in defining the metabolic pathways, the mechanistic action of enzymes, and even the processing of genetic material. The Handbook of Biochemical Kinetics provides the "underlying scaffolding" of logic for kinetic approaches to distinguish rival models or mechanisms. The handbook also comments on techniques and their likely limitations and pitfalls, as well as derivations of fundamental rate equations that characterize biochemical processes. Key Features * Over 750 pages devoted to theory and techniques for studying enzymic and metabolic processes * Over 1,500 definitions of kinetic and mechanistic terminology, with key references * Practical advice on experimental design of kinetic experiments * Extended step-by-step methods for deriving rate equations * Over 1,000 enzymes, complete with EC numbers, reactions catalyzed, and references to reviews and/or assay methods * Over 5,000 selected references to kinetic methods appearing in the Methods in Enzymology series * 72-page Wordfinder that allows the reader to search by keywords * Summaries of mechanistic studies on key enzymes and protein systems * Over 250 diagrams, figures, tables, and structures

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