



Small Molecule Protein Interaction

Sumit Mittal

Small Molecule Protein Interaction:

Targeting Protein-Protein Interactions by Small Molecules Chunquan Sheng, Gunda I. Georg, 2018-06-26 This book comprehensively reviews the state of the art strategies developed for protein protein interaction PPI inhibitors and highlights the success stories in new drug discovery and development Consisting of two parts with twelve chapters it demonstrates the design strategies and case studies of small molecule PPI inhibitors The first part discusses various discovery strategies for small molecule PPI inhibitors such as high throughput screening hot spot based design computational approaches and fragment based design The second part presents recent advances in small molecule inhibitors focusing on clinical candidates and new PPI targets This book has broad appeal and is of significant interest to the pharmaceutical science and medicinal chemistry communities

Small Molecule — Protein Interactions Herbert Waldmann, Marcus Koppitz, 2013-03-09 Based on the international workshop on Small Molecule Protein Interactions held in Berlin April 24 26 2002 researchers from industry and academic laboratories describe novel and efficient ways selecting promising new drug targets and developing small molecule inhibitors against them The structure of the book corresponds to the different aspects of the drug discovery process All chapters are written by leading experts in the field who present and discuss the most recent state of the art tools and techniques for the development of novel drugs The value of the book lies in surveying and summarizing the approaches taken by different companies and institutions giving the reader a balanced view on the use of the latest techniques on the one hand and experience based assistance in selecting appropriate tools for their own work on the other hand

Understanding Small Molecule-protein Interactions Raeanne L. Napoleon, 2012 Abstract The binding of small molecules to a protein is among the most important phenomena in the chemistry of life the activity and functionality of many proteins depend critically on binding small molecules A deep understanding of protein small molecule interactions and the interplay between ligation and function can give valuable insight into key systems of interest The complete characterization of any small molecule protein interaction requires quantification of many interactions and the pursuit of such information is the purpose of this body of work The discovery of binding regions on proteins or hot spots is an important step in drug development To this end a highly regarded and robust fragment based protocol has been developed for the detection of hot spots Firstly we use this protocol in conjunction with other computation techniques such as homology modeling to locate the allosteric binding site of L phenylalanine in Phenylalanine Hydroxylase Secondly computational fragment mapping was employed to locate the site of allostery for Ras an important signaling protein Lastly the identification of hot spots for many unligated protein targets is presented highlighting the importance of a reliable way to predict druggability computationally The second part of this dissertation shifts focus to the development of electrostatic models of small molecules It is widely believed that classical potentials can describe neither vibrational frequency shifts in condensed phases nor the response of vibrational frequencies to an applied electric field the vibrational Stark effect In this work an improved classical molecular

electrostatic model for the CO ligand was developed to faithfully model these phenomena. This model is found to predict the vibrational Stark effect and Fe CO binding energy with unprecedented accuracy for such a classical model. As an extension of this work a geometrically dependent water potential was developed. This work has shown that comparison of results obtained from current water models against experimentally determined proton momentum distributions is an invaluable benchmark.

Protein Surface Recognition Ernest Giralt, Mark Peczuh, Xavier Salvatella, 2011-07-07 A new perspective on the design of molecular therapeutics is emerging. This new strategy emphasizes the rational complementation of functionality along extended patches of a protein surface with the aim of inhibiting protein-protein interactions. The successful development of compounds able to inhibit these interactions offers a unique chance to selectively intervene in a large number of key cellular processes related to human disease. Protein Surface Recognition presents a detailed treatment of this strategy with topics including an extended survey of protein-protein interactions that are key players in human disease and biology and the potential for therapeutics derived from this new perspective. The fundamental physical issues that surround protein-protein interactions that must be considered when designing ligands for protein surfaces examples of protein surface small molecule interactions including treatments of protein natural product interactions, protein interface peptides and rational approaches to protein surface recognition from model to biological systems a survey of techniques that will be integral to the discovery of new small molecule protein surface binders from high throughput synthesis and screening techniques to *in silico* and *in vitro* methods for the discovery of novel protein ligands. Protein Surface Recognition provides an intellectual tool kit for investigators in medicinal and bioorganic chemistry looking to exploit this emerging paradigm in drug discovery.

Protein-Protein Interactions Shahid Mukhtar, 2023-07-14 This detailed volume provides a comprehensive collection of classic and cutting edge methods and techniques in mapping protein-protein interactions. The chapters include a variety of *in vitro* and *in vivo* experimental methods covering cell biology, biochemistry, and biophysics. In addition, the book also explores *in silico* methods including sequence, structure, and phylogenetic profile based approaches as well as gene expression and machine learning methods. Written for the highly successful Methods in Molecular Biology series, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step and readily reproducible laboratory protocols as well as tips on troubleshooting and avoiding known pitfalls. Authoritative and practical Protein Protein Interactions Methods and Protocols serves as an ideal guide for researchers working in protein science and beyond.

Design and Synthesis of Small-molecule Protein-protein Interaction Antagonists Xu Han, 2014 Protein-protein interactions play a crucial role in a wide range of biological processes. Research on the design and synthesis of small molecules to modulate these protein-protein interactions can lead to new targets and drugs to modulate their function. In chapter one we discuss the design and synthesis of small molecules to probe a protein-protein interaction in a voltage-gated Ca₂ channel. Virtual screening identified a compound BTT 3 that contained a 3,4-dihydro-3,4-pyrazole core. This compound

had modest biological activity when tested in a fluorescence polarization FP assay The synthetic route to BTT 3 consisted of six steps In addition analogs of BTT 3 were made for a structure activity study to establish the importance of a carboxylate moiety We also synthesized a biotinylated benzophenone photo affinity probe and linked it to BTT 3 to identify additional protein targets of the compound In Chapter two small molecule antagonists targeting uPA uPAR protein protein interaction are presented A total of 500 commercially available compounds were previously identified by virtual screening and tested by a FP assay Three classes of compounds were found with biological activity The first class of compounds contains pyrrolidone core structures represented by IPR 1110 the second class has a novel pyrrolo 3 4 c pyrazole ring system represented by xv IPR 1283 and the last series had compounds with a 1 2 disubstituted 1 2 dihydropyrrolo 3 4 b indol 3 4H one core structure represented by IPR 540 Each of these three compounds were synthesized and assessed by FP and ELISA assays A binding mode of IPR 1110 with uPA was subsequently proposed Based on this binding mode another 61 IPR 1110 derivatives were synthesized by us to illustrate the SAR activity Analogs of the other two series were also synthesized *Small-Molecule Inhibitors of Protein-Protein Interactions* Lyubomir Vassilev,David Fry,2011-01-18 In this volume the editors have collected the knowledgeable insights of a number of leaders in this field researchers who have achieved success in addressing the difficult problem of inhibiting protein protein interactions These researchers describe their unique approaches and share experiences results thoughts and opinions The content of the articles is rich and in terms of scope ranges from generalized approaches to specific case studies There are various focal points including methodologies and the molecules themselves Ultimately there are numerous lessons to be taken away from this collection and the editors hope that this snapshot of the current state of the art in developing protein protein inhibitors not only pays tribute to the past successes but also generates excitement about the future potential of this field

Cell-Wide Identification of Metabolite-Protein Interactions

Aleksandra Skirycz,Marcin Luzarowski,Jennifer C. Ewald,2022-09-30 This thorough volume explores protocols of proteome and metabolome wide strategies for the identification of protein small molecule complexes in different organisms in order to shed light on these important regulatory interactions Experimental and computational strategies to characterize protein metabolite interactions are discussed and recent advances in enabling technologies are featured as well Written for the highly successful Methods in Molecular Biology series chapters include the kind of detail and expert implementation advice to ensure success in future research Authoritative and practical Cell Wide Identification of Metabolite Protein Interactions will aid researchers seeking a better understanding of the mechanisms of signal transduction occurring in the cell and assessing the effect of complex formation on cell physiology *Protein-Protein Interactions* Michael D. Wendt,2012-06-26 Michael D Wendt Protein Protein Interactions as Drug Targets Shaomeng Wang Yujun Zhao Denzil Bernard Angelo Aguilar Sanjeev Kumar Targeting the MDM2 p53 Protein Protein Interaction for New Cancer Therapeutics Kurt Deshayes Jeremy Murray Domagoj Vucic The Development of Small Molecule IAP Antagonists for the Treatment of Cancer John F Kadow David

R Langley Nicholas A Meanwell Michael A Walker Kap Sun Yeung Richard Pracitto Protein Protein Interaction Targets to Inhibit HIV 1 Infection Nicholas A Meanwell David R Langley Inhibitors of Protein Protein Interactions in Paramyxovirus Fusion a Focus on Respiratory Syncytial Virus Andrew B Mahon Stephen E Miller Stephen T Joy Paramjit S Arora Rational Design Strategies for Developing Synthetic Inhibitors of Helical Protein Interfaces Michael D Wendt The Discovery of Navitoclax a Bcl 2 Family Inhibitor *Molecular Nuclear Medicine* L.E. Feinendegen,W.W. Shreeve,W.C. Eckelman,Yong Whee Bahk,H.N. Jr. Wagner,2012-12-06 Nuclear Medicine techniques have advanced to such a degree that biochemical transparency of the human body has reached the doorstep of medical application The book gives background techniques and examples in an interdisciplinary approach to quantify biochemical reactions *in vivo* by regional imaging and *in vitro* analyses The goal is to assess *in vivo* biochemical homeostatic circuits under control by genes and protein interactions It becomes apparent how nuclear medicine can aid clinical researchers and practitioners human geneticists and pharmacologists in understanding and affecting gene phenotype relationships operating *in vivo* and thus can help eventually to bring functional genomics and proteomics to clinical medicine When Chemistry Meets Biology – Generating Innovative Concepts, Methods and Tools for Scientific Discovery in the Plant Sciences Erich Kombrink,Markus Kaiser,2016-08-12 Biologically active small molecules have increasingly been applied in plant biology to dissect and understand biological systems This is evident from the frequent use of potent and selective inhibitors of enzymes or other biological processes such as transcription translation or protein degradation In contrast to animal systems which are nurtured from drug research the systematic development of novel bioactive small molecules as research tools for plant systems is a largely underexplored research area This is surprising since bioactive small molecules bear great potential for generating new powerful tools for dissecting diverse biological processes In particular when small molecules are integrated into genetic strategies thereby defining chemical genetics they may help to circumvent inherent problems of classical forward genetics There are now clear examples of important fundamental discoveries originating from plant chemical genetics that demonstrate the power but not yet fully exploited potential of this experimental approach These include the unraveling of molecular mechanisms and critical steps in hormone signaling activation of defense reactions and dynamic intracellular processes The intention of this Research Topic of *Frontiers in Plant Physiology* is to summarize the current status of research at the interface between chemistry and biology and to identify future research challenges The research topic covers diverse aspects of plant chemical biology including the identification of bioactive small molecules through screening processes from chemical libraries and natural sources which rely on robust and quantitative high throughput bioassays the critical evaluation and characterization of the compound s activity selectivity and ultimately the identification of its protein target s and mode of action which is yet the biggest challenge of all Such well characterized selective chemicals are attractive tools for basic research allowing the functional dissection of plant signaling processes or for applied purposes if designed for protection of crop plants from disease New

methods and data mining tools for assessing the bioactivity profile of compounds exploring the chemical space for structure function relationships and comprehensive chemical fingerprinting metabolomics are also important strategies in plant chemical biology In addition there is a continuing need for diverse target specific bioprosbes that help profiling enzymatic activities or selectively label protein complexes or cellular compartments To achieve these goals and to add suitable probes and methods to the experimental toolbox plant biologists need to closely cooperate with synthetic chemists The development of such tailored chemicals that beyond application in basic research can modify traits of crop plants or target specific classes of weeds or pests by collaboration of applied and academic research groups may provide a bright future for plant chemical biology The current Research Topic covers the breadth of the field by presenting original research articles methods papers reviews perspectives and opinions

The Molecular Basis of Human Cancer

William B. Coleman, Gregory J. Tsongalis, 2016-11-11 This book covers the concepts of molecular medicine and personalized medicine Subsequent chapters cover the topics of genomics transcriptomics epigenomics and proteomics as the tools of molecular pathology and foundations of molecular medicine These chapters are followed by a series of chapters that provide overviews of molecular medicine as applied broadly to neoplastic genetic and infectious diseases as well as a chapter on molecular diagnostics The volume concludes with a chapter that delves into the promise of molecular medicine in the personalized treatment of patients with complex diseases along with a discussion of the challenges and obstacles to personalized patient care The Molecular Basis of Human Cancer Second Edition is a valuable resource for oncologists researchers and all medical professionals who work with cancer

Methods for Detection of Small Molecule-protein Interactions

Yan Guan, 2015 Detection of molecular interactions is critical for understanding many biological processes for detecting disease biomarkers and for screening drug candidates Fluorescence based approach can be problematic especially when applied to the detection of small molecules Various label free techniques such as surface plasmon resonance technique are sensitive to mass making it extremely challenging to detect small molecules In this thesis novel detection methods for molecular interactions are described First a simple detection paradigm based on reflectance interferometry is developed This method is simple low cost and can be easily applied for protein array detection Second a label free charge sensitive optical detection CSOD technique is developed for detecting of both large and small molecules The technique is based on that most molecules relevant to biomedical research and applications are charged or partially charged An optical fiber is dipped into the well of a microplate It detects the surface charge of the fiber which does not decrease with the size mass of the molecule making it particularly attractive for studying small molecules Third a method for mechanically amplification detection of molecular interactions MADMI is developed It provides quantitative analysis of small molecules interaction with membrane proteins in intact cells The interactions are monitored by detecting a mechanical deformation in the membrane induced by the molecular interactions With this novel method small molecules and membrane proteins interaction in the intact cells can be detected

This new paradigm provides mechanical amplification of small interaction signals allowing us to measure the binding kinetics of both large and small molecules with membrane proteins and to analyze heterogeneous nature of the binding kinetics between different cells and different regions of a single cell. Last by tracking the cell membrane edge deformation binding caused downstream event granule secretory has been measured. This method focuses on the plasma membrane change when granules fuse with the cell. The fusion of granules increases the plasma membrane area and thus the cell edge expands. The expansion is localized at the vesicle release location. Granule size was calculated based on measured edge expansion. The membrane deformation due to the granule release is real time monitored by this method.

Studies on Small Molecule-protein Interactions with a Note on the Use of Tracers in Transport Systems Erik Olof Arvidsson, 1965

Inhibitors of Protein-Protein Interactions Ali Tavassoli, 2020-11-25 Protein protein interactions PPI are at the heart of the majority of cellular processes and are frequently dysregulated or usurped in disease. Given this central role the inhibition of PPIs has been of significant interest as a means of treating a wide variety of diseases. However there are inherent challenges in developing molecules capable of disrupting the relatively featureless and large interfacial areas involved. Despite this there have been a number of successes in this field in recent years using both traditional drug discovery approaches and innovative interdisciplinary strategies using novel chemical scaffolds. This book comprehensively covers the various aspects of PPI inhibition encompassing small molecules peptidomimetics cyclic peptides stapled peptides and macrocycles. Illustrated throughout with successful case studies this book provides a holistic cutting edge view of the subject area and is ideal for chemical biologists and medicinal chemists interested in developing PPI inhibitors.

Using Protein-protein Interactions to Influence Small Molecule Activity Patrick Dale Braun, 2003 *Studies on Small Molecule - Protein Interactions in Transport Systems* Erik Olof Arvidsson, 1965

Studies on small molecule - protein interactions with a note on the use of tracers in transport systems Erik Olof Arvidsson, 1965

Protein Targeting with Small Molecules Hiroyuki Osada, 2009-07-31 Discover the link between the latest chemical biology approaches and novel drug therapies. *Protein Targeting with Small Molecules Chemical Biology Techniques and Applications* takes readers beyond the use of chemical biology in basic research providing a highly relevant look at techniques that can address the challenges of biology and drug design and development. This indispensable bench companion features up to date coverage of advances in chemistry and assesses their impact on developing new therapeutics making it ideal for chemical biologists and medicinal chemists who are developing small molecule drugs to target proteins and treat diseases. In addition the book examines the full range of complex biological systems and their interrelationship with chemistry from the interaction of biological response modifiers with proteins to the chemical biology of cell surface oligosaccharides. Distinguished by an overview of chemical biology that is reinforced and clarified by detailed examples and descriptions of techniques. *Protein Targeting with Small Molecules Chemical Biology Techniques and Applications* introduces key technologies and methods of chemical biology designed to

detect the interactions of small molecules and proteins Facilitates the discovery of small molecules that bind to proteins and describes the molecules application in the investigation of biological processes Presents timely coverage of the development of fluorescent probes for small molecules as well as the generation of small molecule ligands and inhibitors Reviews important techniques such as chemical genomics target profiling immobilization technology detection methods chemical inhibition and structure based targeting Offers a compelling synopsis of data that underscores the recent progress made in the area of targeting proteins by small molecules **Small Molecule Modulation of Protein-protein Interactions** Sumit Mittal,2017

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