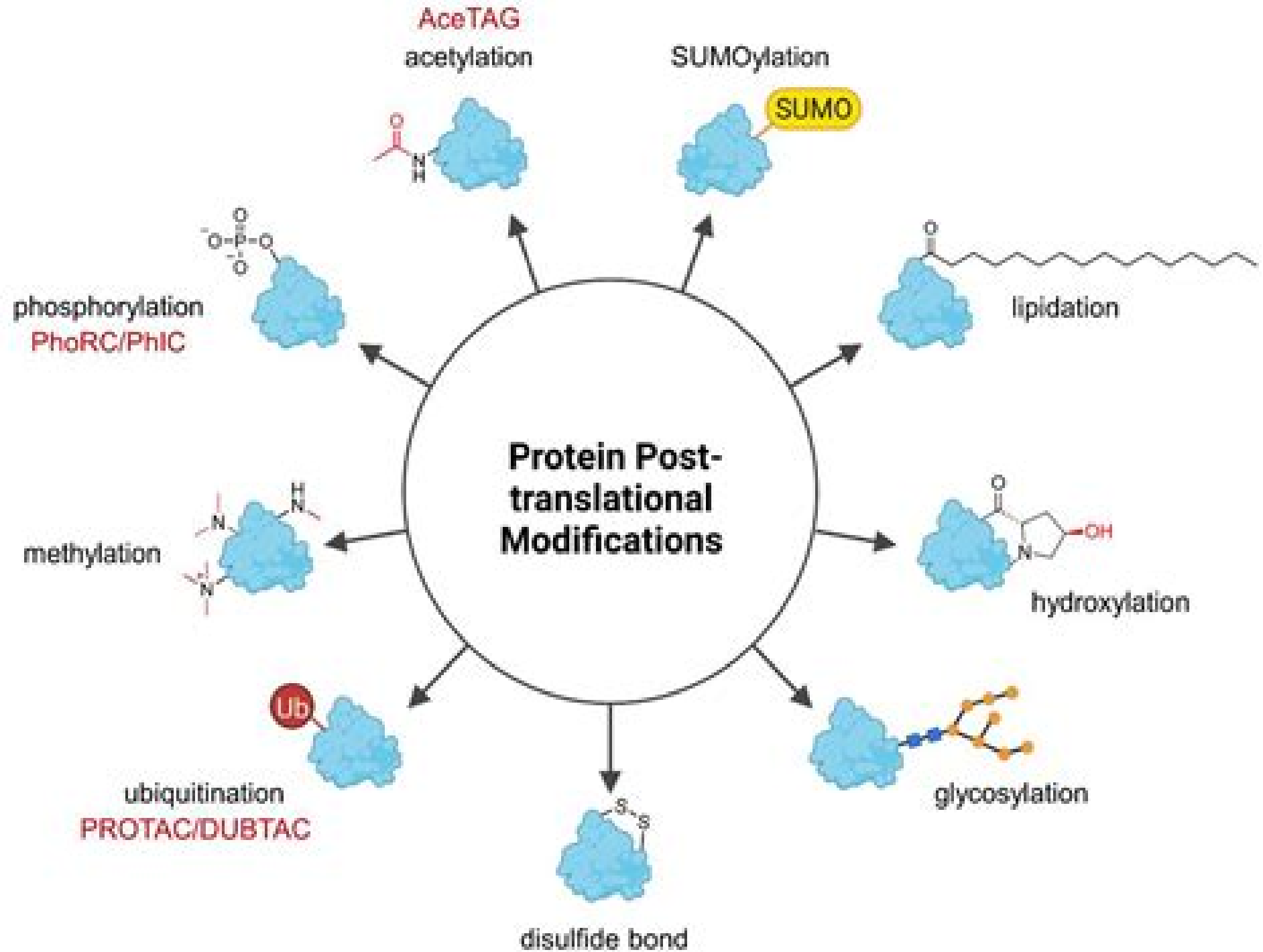




Small Molecule Protein Interaction

Xu Han



Small Molecule Protein Interaction:

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

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 *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

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 proteinprotein 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 proteinprotein 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-yl 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

Protein Surface Recognition Ernest Giralt, Mark Pecuh, 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 Interactions as Targets in Drug Discovery Rossen Donev, 2020-04-18 Protein Interactions as Targets in Drug Discovery Volume 121 is dedicated to the design of therapeutics both experimental and computational that target protein interactions Chapters in this new release include Trends in structure based drug design with protein targets From fragment to peptide protein interaction addressing the structural basis of binding using Supervised Molecular Dynamics SuMD Protein protein and protein ligand interactions identification of potential inhibitors through computational analysis Aromatic aromatic interactions in protein drug and protein protein interactions Role of protein protein interaction in allosteric drug design within the human methyltransferase and much more Integrates experimental and computational methods for studying protein interactions and their modulation by potential therapeutics Contains timely chapters written by well renowned authorities in their field Covers information that is well supported by a number of high quality illustrations figures and tables Targets a very wide audience of specialists researchers and students

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

Protein Interactions Peter Schuck,2007-03-20 When I was invited to edit this volume I wanted to take the opportunity to assemble reviews of different biophysical methodologies for protein interactions at a level sufficiently detailed to understand how complex systems can be studied There are several excellent introductory texts for biophysical methodologies many with hands on descriptions or embedded in general introductions to physical chemistry The goal of the present volume was to present state of the art reviews that do not necessarily enable the reader to carry out these techniques but to gain a deep understanding of the biophysical observables to stimulate creative thought on how the techniques may be applied to study a particular biological system and to foster collaboration and multidisciplinary work Reversible protein interactions involve noncovalent chemical bonds producing protein complexes with free energies not far from the order of magnitude of the thermal energy kT As a consequence they can be highly dynamic and may be controlled for example by protein expression levels and changes in the intracellular or microenvironment Reversible protein complexes may have sufficient stability to be purified for study but frequently their short lifetime essentially limits their existence to solutions of mixtures of the binding partners in which they remain populated through dissociation and reassociation processes To understand the function of such protein complexes it is important to study their structure and dynamics

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