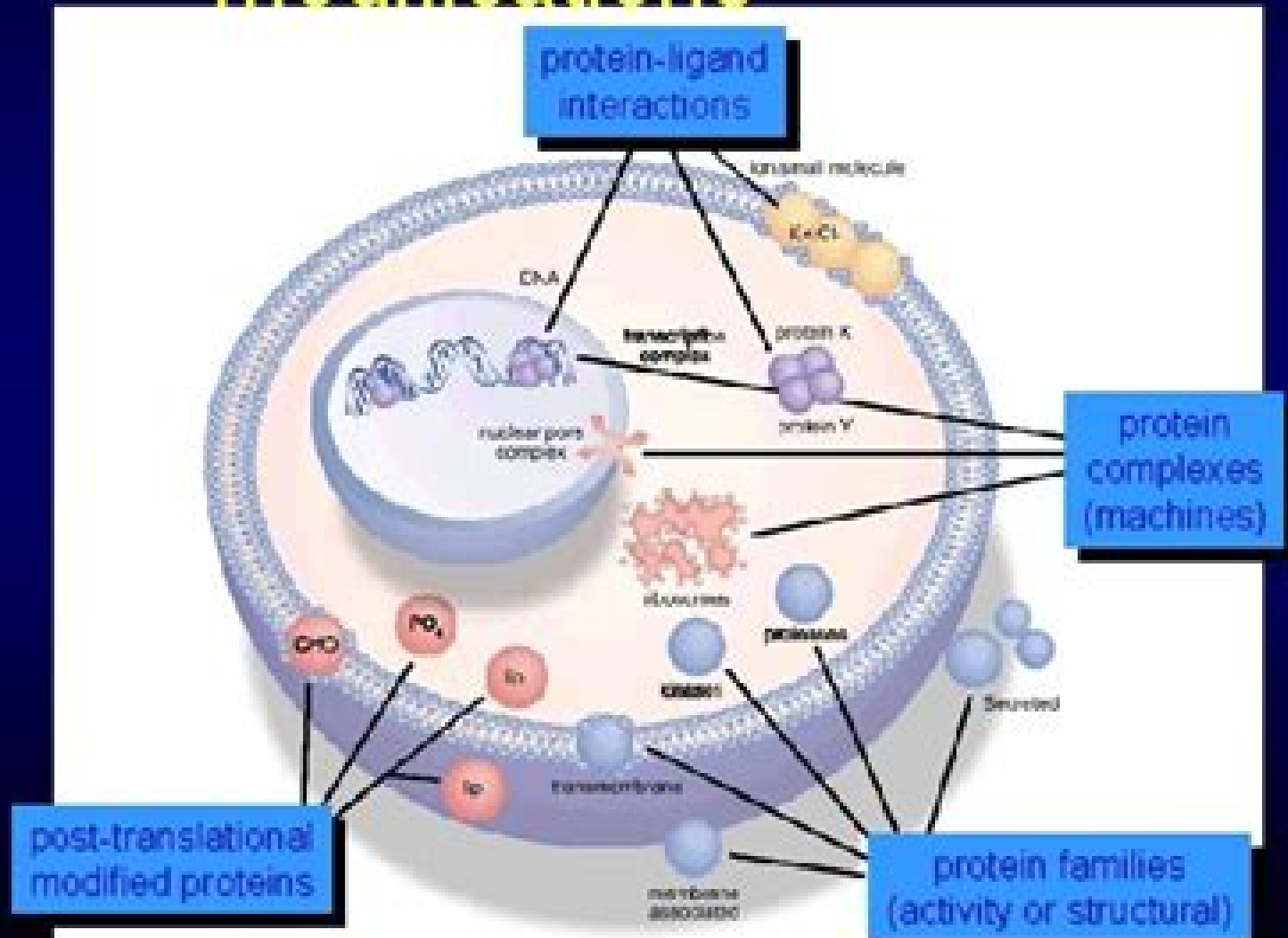


Proteomics and posttranslational modifications



Patterson and Aebersold, Nature Genetics (supp.), 33, 311 (2003)

Proteinligand Interactions

Holger Gohlke



Proteinligand Interactions:

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Protein-Ligand Interactions Holger Gohlke, 2012-05-21 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

Protein-ligand Interactions, Structure and Spectroscopy Stephen E. Harding, Babur Z. Chowdhry, 2001 This text on protein ligand interactions offers a selection of the most useful and easily applied methods and acts as a guide to the principal techniques used

Protein-Ligand Interactions Hans-Joachim Böhm, Gisbert Schneider, 2003-05-06 Protein-ligand Interactions Horst Sund, Gideon Blauer, 1975 Keine ausführliche Beschreibung für Protein Ligand Interactions verfügbar

Understanding

protein-ligand interactions Charles H. Reynolds, 2006

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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

Understanding Protein-ligand Interactions Sunil Patel, 1998

Protein-ligand Interactions Stephen E. Harding, Babur

Z. Chowdhry, 2001

Recent Developments on Protein-Ligand Interactions Alexandre G de Brevern, 2022-03-21

Protein ligand interactions play a fundamental role in most major biological functions The number and diversity of small molecules that interact with proteins whether naturally or not can quickly become overwhelming They are as essential as amino acids nucleic acids or membrane lipids enabling a large number of essential functions One need only think of carbohydrates or even just ATP to be certain They are also essential in drug discovery With the increasing structural information of proteins and protein ligand complexes molecular modelling molecular dynamics and chemoinformatics approaches are often required for the efficient analysis of a large number of such complexes and to provide insights Similarly numerous computational approaches have been developed to characterize and use the knowledge of such interactions which can lead to drug candidates Recent Developments on Protein Ligand Interactions From Structure Function to Applications was dedicated to the different aspect of protein ligand analysis and or prediction using computational approaches as well as new developments dedicated to these tasks It will interest both specialists and non specialists as the presented studies cover a very large spectra in terms of methodologies and applications It underlined the variety of scientific area linked to these questions i e chemistry biology physics informatics bioinformatics structural bioinformatics and chemoinformatics

Protein-ligand Interactions Stephen E. Harding, Babur Z. Chowdhry, 2001 The two Practical Approach volumes provide a selection of the most useful and easily applied methods and will be an invaluable guide to the principle techniques used to study the interactions of proteins and ligands The first volume covers the principal hydrodynamic and calorimetric techniques for studying protein ligand interactions The second volume covers all the principal spectroscopic and structural methods for investigating protein ligand interactions

Computational Intelligence in Protein-Ligand Interaction Analysis Bing

Wang, Peng Chen, Jun Zhang, 2024-03-22

Computational Intelligence in Protein Ligand Interaction Analysis presents computational techniques for predicting protein ligand interactions recognizing protein interaction sites and identifying

protein drug targets The book emphasizes novel approaches to protein ligand interactions including machine learning and deep learning presenting a state of the art suite of skills for researchers The volume represents a resource for scientists detailing the fundamentals of computational methods showing how to use computational algorithms to study protein interaction data and giving scientific explanations for biological data through computational intelligence Fourteen chapters offer a comprehensive guide to protein interaction data and computational intelligence methods for protein ligand interactions Presents a guide to computational techniques for protein ligand interaction analysis Guides researchers in developing advanced computational intelligence methods for the protein ligand problem Identifies appropriate computational tools for various problems Demonstrates the use of advanced techniques such as vector machine neural networks and machine learning Offers the computational mathematical and statistical skills researchers need Protein-ligand Interactions Stephen E. Harding, Babur Z. Chowdhry, 2001

An Investigation Into the Role of Protein-ligand Interactions on Obligate and Transient Protein-protein Interactions [microform] Quinlan, Robert Jason, 2005 Protein ligand and protein protein interactions are critical to cellular function Most cellular metabolic and signal transduction pathways are influenced by these interactions consequently molecular level understanding of these associations is an important area of biochemical research We have examined the thermodynamics of several protein protein associations and the protein ligand interactions that mediate them Using Fluorescence Correlation Spectroscopy we have examined the putative interaction between pig heart malate dehydrogenase MDH and citrate synthase CTS We demonstrate a specific low affinity interaction between these enzymes The association is highly polyethylene glycol PEG dependent and at high concentrations of NaCl or PEG non specific aggregates are formed We demonstrate that oxaloacetate the intermediate common to both CTS and MDH induces the association at concentrations below the K_m of CTS suggesting that the open conformation of CTS is involved in the association Using several biophysical techniques we have examined the subunit associations of *B. stearothermophilus* phosphofructokinase PFK We demonstrate that the inhibitor bound conformation of the enzyme has reduced subunit affinity The kinetics and thermodynamics of the phosphoenolpyruvate PEP induced dissociation of PFK have been quantified Binding substrate fructose 6 phosphate F6P stabilizes the enzyme to inhibitor induced dissociation by 132 fold These data suggest that subunit associations may play a role in the allosteric inhibition of PFK by PEP The thermodynamics of the protein ligand associations and allosteric inhibition of *E. coli* phosphofructokinase have been examined using intrinsic fluorescence and hydrostatic pressure Both ligand binding affinity and PEP inhibition are diminished by pressure whereas substrate binding affinity for inhibitor bound enzyme is pressure insensitive Larger entropic than enthalpic changes with pressure lead to the overall reduction in free energies Using a fluorescence based assay we have developed a series of baroresistant buffer mixtures By combining a buffer with acid dissociation of negative volume with a buffer of positive volume a pressure resistant mixture is produced Alteration of the molar ratio of the two component buffers

yields mixtures that are pressure insensitive at pH values around neutrality *DNA-Ligand Interactions W.*

Guschlbauer, Wolfram Saenger, 1987-08 This volume contains the texts of the nineteen lectures presented at the NATO ASI FEBS Course on DNA ligand interactions from drugs to proteins The Advanced Study Institute ASI was held from August 30th to September 11th 1986 in the Abbey of Fontevraud France The ASI was attended by 112 participants from a wide scientific horizon and from twentyone different countries It was in some way a follow up of the ASI held in Maratea Italy in May 1981 and which was published in the NATO ASI Life Science series as volume 45 While much has been learned about the way the cellular machinery maintains and transmits the genetic heritage as well as how these processes are regulated little is known about how the interactions between the various partners involved are taking place The interactions of drugs and proteins with nucleic acids are of evident importance in the understanding of these problems The spectacular advances in recombinant DNA technology and the increased sophistication of biophysical techniques in particular ray diffraction and nuclear magnetic resonance have created a scientific environment which is highly promising for the future of research in molecular biology These advances permit the serious hope that biology on the molecular level may become a reality Some of the contributions at the ASI presented the most recent advances in this exciting field **Recent Developments on**

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acid PMPA a degradation product of the nerve agent soman The computationally redesigned binding proteins were labeled with a thiolreactive fluorophore at a unique cysteine position and as a result a change in fluorescence is exhibited by the protein fluorophore conjugate in response to ligand binding The results demonstrate that the engineered proteins act as reagentless fluorescent biosensors for PMPA and exhibit a range of affinities between 0.045 and 10 μ M Protein engineering techniques were used to extent the ability of a single biosensor element to distinguish between several similar target ligands by incorporating many sensor elements in a multisensor system The protein PhnD a periplasmic binding protein that binds many phosphonates was characterized and variants were constructed by introducing point mutations in its binding pocket The PhnD variants exhibit differential binding affinities to several similar molecules and were used as sensor elements in a fluorescent multisensor system The multisensor can be used to determine the concentrations of many analytes in a solution and can detect the presence of an interferent for which it has not been characterized by taking advantage of the non linear nature of the fluorescent response to ligand binding

Modeling Protein Ligand Interactions Using Multi-scale Computational Approaches Ashini Bolia, 2015 Molecular docking serves as an important tool in modeling protein ligand interactions Most of the docking approaches treat the protein receptor as rigid and move the ligand in the binding pocket through an energy minimization which is an incorrect approach as proteins are flexible and undergo conformational changes upon ligand binding However modeling receptor backbone flexibility in docking is challenging and computationally expensive due to the large conformational space that needs to be sampled A novel flexible docking approach called BP Dock Backbone Perturbation docking was developed to overcome this challenge BP Dock integrates both backbone and side chain conformational changes of a protein through a multi scale approach In BP Dock the residues along a protein chain are perturbed mimicking the binding induced event with a small Brownian kick one at a time The fluctuation response profile of the chain upon these perturbations is computed by Perturbation Response Scanning PRS to generate multiple receptor conformations for ensemble docking To evaluate the performance of BP Dock this approach was applied to a large and diverse dataset of unbound structures as receptors Furthermore the protein peptide docking of PICK1 PDZ proteins was investigated This study elucidates the determinants of PICK1 PDZ binding that plays crucial roles in numerous neurodegenerative disorders BP Dock approach was also extended to the challenging problem of protein glycan docking and applied to analyze the energetics of glycan recognition in Cyanovirin N CVN a cyanobacterial lectin that inhibits HIV by binding to its highly glycosylated envelope protein gp120 This study provide the energetic contribution of the individual residues lining the binding pocket of CVN and explore the effect of structural flexibility in the hinge region of CVN on glycan binding which are also verified experimentally Overall these successful applications of BP Dock highlight the importance of modeling backbone flexibility in docking that can have important implications in defining the binding properties of protein ligand interactions Finally an induced fit docking approach called Adaptive BP Dock is presented that allows both protein and

ligand conformational sampling during the docking Adaptive BP Dock can provide a faster and efficient docking approach for the virtual screening of novel targets for rational drug design and aid our understanding of protein ligand interactions

Computational Analyses of Protein-ligand Interactions ,2010

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