

Protein Dynamics, Function, and Design

Oleg Jardetzky and Jean-François Lefèvre

NATO ASI Series

Protein Dynamics Function And Design

Timir Tripathi, Vikash Kumar Dubey

Protein Dynamics Function And Design:

Protein Dynamics, Function, and Design Oleg Jardetzky, Jean-François Lefèvre, 2012-12-06 This volume is a collection of articles from the proceedings of the International School of Structural Biology and Magnetic Resonance 3rd Course Protein Dynamics Function and Design This NATO Advance Study Institute was held in Erice at the Ettore Majorana Centre for Scientific Culture on April 16 28 1997 The aim of the Institute was to bring together experts applying different physical methods to problems of macro molecular dynamics notably x ray diffraction NMR and other forms of spectroscopy and molecular dynamics simulations Emphasis was placed on those systems and types of problems such as mechanisms of allosteric control signal transmission induced fit to different ligands with its implications for drug design and the effects of dynamics on structure determination where a correlation of findings obtained by different methods could shed the most light on the mechanisms involved and stimulate the search for new approaches The individual articles represent the state of the art in each of the areas covered and provide a guide to the original literature in this rapidly developing field v CONTENTS 1 Determining Structures of ProteinlDN A Complexes by NMR Angela M Gronenbom and G Marius Clore 2 Fitting Protein Structures to Experimental Data Lessons from before Your Mother Was Born 15 Jeffrey C Hoch Alan S Stem and Peter J Connolly 3 Multisubunit Allosteric Proteins 27 William N Lipscomb 4 Studying Protein Structure and Function by Directed Evolution Examples with Engineered Antibodies 37Andreas Pliickthun 5 High Pressure Effects on Protein Structure Protein Sequence to Motion to Function Adam Damry, 2019 Protein dynamics are critical to the structure and function of proteins However due to the complexity they inherently bring to the protein design problem dynamics historically have not been considered in computational protein design CPD Herein we present meta MSD a new CPD methodology for the design of protein dynamics We applied our methodology to the design of a novel mode of conformational exchange in Streptococcal protein G domain B1 producing dynamic variants we termed DANCERs Predictions were validated by NMR characterization of selected DANCERs confirming that our meta MSD framework is suitable for the computational design of protein dynamics We then performed a thorough NMR characterization of the sequence determinants of dynamics in one DANCER isolating two mutations responsible for the novel dynamics this protein exhibits The first A34F is responsible for destabilizing the highly stable native G 1 conformation allowing the protein to sample other conformational states The second V39L mediates subtle interactions that stabilize the designed conformational trajectory in the context of the A34F mutation Together these results highlight the role of protein plasticity in the development of dynamics and the need for highly accurate computational tools to approach similar design problems Finally we present an NMR based characterization of structural dynamics in a family of related red fluorescent proteins RFPs and pinpoint regions of the RFP structure where dynamics correlate to RFP brightness This overview of the RFP dynamics function relationship will be used in future projects to perform a computation design of functional dynamics in RFPs Computational Approaches to Protein Dynamics Monika Fuxreiter, 2014-12-24 The Latest Developments on the Role of Dynamics in Protein FunctionsComputational Approaches to Protein Dynamics From Quantum to Coarse Grained Methods presents modern biomolecular computational techniques that address protein flexibility dynamics at all levels of theory An international contingent of leading researchers in chemistry physics an Structural and Dynamic Aspects of Protein Function and Allostery George Lisi, Ivan Rivalta, Vincenzo Venditti, 2022-03-28 Invitation to Protein Sequence Analysis Through Probability and Information Daniel J. Graham, 2019-02-06 This book explores the remarkable information correspondences and probability structures of proteins Correspondences are pervasive in biochemistry and bioinformatics proteins share homologies folding patterns and mechanisms Probability structures are just as paramount folded state graphics reflect Angstrom scale maps of electron density The author explores protein sequences primary structures both individually and in sets systems with the help of probability and information tools This perspective will enhance the reader s knowledge of how an important class of molecules is designed and put to task in natural systems and how we can approach class members in hands on ways

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Computational Genomics and Structural Bioinformatics in Microbial Science Javid Ahmad Parray, Niraj Singh, Wen-Jun Li, 2025-02-24 Computational Genomics and Structural Bioinformatics in Microbial Science Microbial Genomics Volume 2 covers different aspects of microbial genomics metagenomics and functional studies of microbes through informative illustrations of current trends in computational tools and bioinformatics approach in environmental microbiology and clinical diagnosis. This book aims to provide readers with an overview of the microbial genome computational genomics and structural bioinformatics in microbial science as well as the most recent developments in these fields This book covers a range of topics including the challenges and opportunities of computational epigenomics bioinformatics tools for assessing metagenomic data as well as computed comparative genomics and computational phenotyping of microorganisms relevant to agriculture Microbial Genomics Host Adaptation virulence and Evolution is a valuable resource for faculty members researchers and undergraduate and postgraduate students at universities medical research labs that are interested in microbial science specifically related to the microbial genome computing genomics and bioinformatics Provides informative illustrations of current trends in computational tools and bioinformatics approach Presents bioinformatics of next generation sequencing in clinical microbiology diagnosis Discusses structural bioinformatics and its applications **Explorations in Computational Physics** Devang Patil, 2025-02-20 Explorations in Computational Physics delves into the intricate world of computational physics offering a comprehensive guide from fundamental theories to cutting edge applications This book serves as an indispensable companion for both novice learners and seasoned researchers We cover a diverse array of topics meticulously unfolding layers of computational techniques and their applications in various branches of physics From classical mechanics simulations elucidating celestial mechanics to quantum mechanics computations unraveling atomic and subatomic realms the book navigates through the vast landscape of computational methodologies with clarity and precision

Furthermore we delve into electromagnetic field simulations statistical mechanics and thermodynamics equipping readers with tools to model complex physical phenomena with accuracy and efficiency High performance computing techniques data analysis and visualization methodologies are elucidated empowering readers to harness modern computational resources in their research With lucid explanations illustrative examples and insightful discussions on emerging technologies like quantum computing and artificial intelligence Explorations in Computational Physics fosters a deeper understanding of computational methodologies and their transformative impact on physics research On protein structure, function and modularity from an evolutionary perspective Robert Pilstål, 2018-05-23 We are compounded entities given life by a complex molecular machinery. When studying these molecules we have to make sense of a diverse set of dynamical nanostructures with wast and intricate patterns of interactions Protein polymers is one of the major groups of building blocks of such nanostructures which fold up into more or less distinct three dimensional structures Due to their shape dynamics and chemical properties proteins are able to perform a plethora of specific functions essential to all known cellular lifeforms The connection between protein sequence translated into protein structure and in the continuation into protein function is well accepted but poorly understood Malfunction in the process of protein folding is known to be implicated in natural aging cancer and degenerative diseases such as Alzheimer's Protein folds are described hierarchically by structural ontologies such as SCOP CATH and Pfam all which has yet to succeed in deciphering the natural language of protein function These paradigmatic views centered on protein structure fail to describe more mutable entities such as intrinsically disordered proteins IDPs which lack a clear defined structure As of 2012 about two thirds of cancer patients was predicted to survive past 5 years of diagnosis Despite this about a third do not survive and numerous of successfully treated patients suffer from secondary conditions due to chemotherapy surgery and the like In order to handle cancer more efficiently we have to better understand the underlying molecular mechanisms Elusive to standard methods of investigation IDPs have a central role in pathology dysfunction in IDPs are key factors in cellular system failures such as cancer as many IDPs are hub regulators for major cell functions These IDPs carry short conserved functional boxes that are not described by known ontologies which suggests the existence of a smaller entity In an investigation of a pair of such boxes of c MYC a plausible structural model of its interacting with Pin1 emerged but such a model still leaves the observer with a puzzle of understanding the actual function of that interaction If the protein is represented as a graph and modeled as the interaction patterns instead of as a structural entity another picture emerges As a graph there is a parable from that of the boxes of IDPs to that of sectors of allosterically connected residues and the theory of foldons and folding units Such a description is also useful in deciphering the implications of specific mutations In order to render a functional description feasible for both structured and disordered proteins there is a need of a model separate from form and structure Realized as protein primes patterns of interaction which has a specific function that can be defined as prime interactions and context With function defined as interactions it might be

possible that the discussion of proteins and their mechanisms is thereby simplified to the point rendering protein structural determination merely supplementary to understanding protein function M nniskan byggs upp av celler de i sin tur best r av n mindre best ndsdelar livets molekyler Dessa fungerar som mekaniska byggstenar likt maskiner och robotar som sliter vid fabrikens band envar utf randes en absolut n dv ndig funktion f r cellens och hela kroppens fortsatta verlevnad De av livets molekyler som beskrivs centralt i den hr avhandling r proteiner vilka i sin tur best r utav en l ng kedja med olika typer av l nkar som likt garn lindar upp sig i ett nystan av en mer eller mindre best md struktur som avg r dess roll och funktion i cellen Intrinsiellt oordnade proteiner IDP gremot denna enklask dning der proteiner som saknar struktur och beter sig mer likt spaghetti i vatten n en maskin IDP r nd funktionella och b r p centrala roller i cellens maskineri exempel r oncoproteinet c Myc som agerar gaspedal fr cellen fel i c Myc s funktion leder till att cellerna l per amok delar sig hejdl st och vi fr cancer Man har uppt ckt att c Myc har en ombytlig struktur vi inte kan se studier av punktvisa f r ndringar mutationer i kedjan av byggstenar hos c Myc visar att m nga l nkar har viktiga roller i funktionen Detta ger oss b ttre f rst else om cancer men samtidigt r laboratoriearbetet b de komplicerat och dyrt h r kan evolutionen v gleda oss och avsl ja hemligheterna snabbare Molekyl r evolution studeras genom att ber kna variation i proteinkedjan mellan besl ktade arter som finns lagrade i databaser detta visar snabbt via n tverksanalys och grafteori vilka delar av proteinet som r centrala och kopplade till varandra av n dv ndighet f r artens fortlevnad P s vis hj lper evolutionen oss att f rst proteinfunktioner via modeller baserade p proteinernas interaktioner snarare n deras struktur Samma modeller kan nyttjas f r att f rst dynamiska f rlopp och skillnader mellan normala och patologiska varianter av proteiner mutationer kan uppst i v r arvsmassa som kan leda till sjukdom Genom analys av proteinernas kopplingsn tverk i grafmodellerna kan man b ttre f ruts ga vilka mutationer som r farligare n andra Dessutom har det visat sig att en s dan representation kan ge b ttre f rst else f r den normala funktionen hos ett protein n vad en proteinstruktur kan H r introduceras ven konceptet proteinprim rer vilket r en abstrakt representation av proteiner centrerad p deras interaktiva m nster snarare n p partikul r form och struktur Det r en f rhoppning att en s dan representation skall f renkla diskussionen anbelangande proteinfunktion s till den grad att strukturbest mmelse av proteiner som r en mycket kostsam och tidskr vande process till viss m n kan anses vara sekund r i betydelse j mf rt med funktionellt modellerande baserat p evolution ra data extraherade ur v ra sekvensdatabaser

Biomedical Index to PHS-supported Research: pt. A. Subject access A-H ,1994 Advances in Protein Molecular and Structural Biology Methods Timir Tripathi, Vikash Kumar Dubey, 2022-01-14 Advances in Protein Molecular and Structural Biology Methods offers a complete overview of the latest tools and methods applicable to the study of proteins at the molecular and structural level The book begins with sections exploring tools to optimize recombinant protein expression and biophysical techniques such as fluorescence spectroscopy NMR mass spectrometry cryo electron microscopy and X ray crystallography It then moves towards computational approaches considering structural bioinformatics

molecular dynamics simulations and deep machine learning technologies. The book also covers methods applied to intrinsically disordered proteins IDPs followed by chapters on protein interaction networks protein function and protein design and engineering. It provides researchers with an extensive toolkit of methods and techniques to draw from when conducting their own experimental work taking them from foundational concepts to practical application. Presents a thorough overview of the latest and emerging methods and technologies for protein study Explores biophysical techniques including nuclear magnetic resonance X ray crystallography and cryo electron microscopy Includes computational and machine learning methods. Features a section dedicated to tools and techniques specific to studying intrinsically disordered proteins

Protein Engineering Handbook Stefan Lutz, Uwe Theo Bornscheuer, 2012-07-31 Unparalleled in size and scope this new major reference integrates academic and industrial knowledge into a single resource allowing for a unique overview of the entire field Adopting a systematic and practice oriented approach and including a wide range of technical and methodological information this highly accessible handbook is an invaluable toolbox for any bioengineer In two massive volumes it covers the full spectrum of current concepts methods and application areas Biomass, Biofuels, Biochemicals Sudhir P. Singh, Ashok Pandey, Reeta Rani Singhania, Christian Larroche, Zhi Li, 2020-04-03 Advances in Enzyme Catalysis and Technologies intends to provide the basic structural and functional descriptions and classification of enzymes The scientific information related to the recombinant enzyme modifications discovery of novel enzymes and development of synthetic enzymes are also presented The translational aspects of enzyme catalysis and bioprocess technologies are illustrated by emphasizing the current requirements and future perspectives of industrial biotechnology Several case studies are included on enzymes for biofuels application micro algal biorefineries high value bioactive molecules production and enzymes for environmental processes such as enzymatic bioprocessing for functional food development biocatalytic technologies for the production of functional sweetener etc Provides a conceptual understanding of enzyme catalysis enzyme engineering discovery of novel enzymes and technology perspectives Includes comprehensive information about the inventions and advancement in enzyme system development for biomass processing and functional food developmental aspects Gives an updated reference for education and understanding of enzyme technology Focus on Protein Research John W. Robinson, 2004 Protein research is a frontier field in science Proteins are widely distributed in plants and animals and are the principal constituents of the protoplasm of all cells and consist essentially of combinations of a amino acids in peptide linkages Twenty different amino acids are commonly found in proteins and serve as enzymes structural elements hormones immunoglobulins etc and are involved throughout the body and in photosynthesis This new book gathers new leading edge research from throughout the world in this exciting and exploding field of research **Biomolecular Simulations in** Structure-Based Drug Discovery Francesco L. Gervasio, Vojtech Spiwok, Raimund Mannhold, 2019-04-29 A guide to applying the power of modern simulation tools to better drug design Biomolecular Simulations in Structure based Drug

Discovery offers an up to date and comprehensive review of modern simulation tools and their applications in real life drug discovery for better and quicker results in structure based drug design The authors describe common tools used in the biomolecular simulation of drugs and their targets and offer an analysis of the accuracy of the predictions They also show how to integrate modeling with other experimental data Filled with numerous case studies from different therapeutic fields the book helps professionals to quickly adopt these new methods for their current projects Experts from the pharmaceutical industry and academic institutions present real life examples for important target classes such as GPCRs ion channels and amyloids as well as for common challenges in structure based drug discovery Biomolecular Simulations in Structure based Drug Discovery is an important resource that Contains a review of the current generation of biomolecular simulation tools that have the robustness and speed that allows them to be used as routine tools by non specialists Includes information on the novel methods and strategies for the modeling of drug target interactions within the framework of real life drug discovery and development Offers numerous illustrative case studies from a wide range of therapeutic fields Presents an application oriented reference that is ideal for those working in the various fields Written for medicinal chemists professionals in the pharmaceutical industry and pharmaceutical chemists Biomolecular Simulations in Structure based Drug Discovery is a comprehensive resource to modern simulation tools that complement and have the potential to complement or replace laboratory assays for better results in drug design Reviews in Computational Chemistry, Volume 2 Kenny B. Lipkowitz, Donald B. Boyd, 2009-09-22 This second volume of the series Reviews in Computational Chemistry explores new applications new methodologies and new perspectives. The topics covered include conformational analysis protein folding force field parameterizations hydrogen bonding charge distributions electrostatic potentials electronic spectroscopy molecular property correlations and the computational chemistry literature Methodologies described include conformational search strategies distance geometry molecular mechanics molecular dynamics ab initio and semiempirical molecular orbital calculations and quantitative structure activity relationships QSAR using topological and electronic descriptors A compendium of molecular modeling software will help users select the computational tools they need Each chapter in Reviews in Computational Chemistry serves as a brief tutorial for organic physical pharmaceutical and biological chemists new to the field Practitioners will be interested in the recent advances Crystallography of Protein Dynamics, 2023-09-25 Research Awards Index ,1989 Approx 400 pagesApprox 400 pages Structural Biology in Drug Discovery Jean-Paul Renaud, 2020-01-27 With the most comprehensive and up to date overview of structure based drug discovery covering both experimental and computational approaches Structural Biology in Drug Discovery Methods Techniques and Practices describes principles methods applications and emerging paradigms of structural biology as a tool for more efficient drug development Coverage includes successful examples academic and industry insights novel concepts and advances in a rapidly evolving field The combined chapters by authors writing from the frontlines of structural biology and drug discovery

give readers a valuable reference and resource that Presents the benefits limitations and potentiality of major techniques in the field such as X ray crystallography NMR neutron crystallography cryo EM mass spectrometry and other biophysical techniques and computational structural biology Includes detailed chapters on druggability allostery complementary use of thermodynamic and kinetic information and powerful approaches such as structural chemogenomics and fragment based drug design Emphasizes the need for the in depth biophysical characterization of protein targets as well as of therapeutic proteins and for a thorough quality assessment of experimental structures Illustrates advances in the field of established therapeutic targets like kinases serine proteinases GPCRs and epigenetic proteins and of more challenging ones like protein protein interactions and intrinsically disordered proteins Magnetic Tweezers for the Study of Protein Structure and Function, 2024-03-14 Magnetic Tweezers for the Study of Protein Structure and Function Volume 694 in the Methods in Enzymology serial highlights new advances in the field with this new volume presenting interesting chapters on a variety of topics including Single membrane protein tethering for magnetic tweezer experiments Membrane protein folding studies using a robust magnetic tweezer method Magnetic tweezers in cell mechanics and more Provides the authority and expertise of leading contributors from an international board of authors Presents the latest release in the Methods in Enzymology serials Updated release includes the latest information on Magnetic Tweezers for the Study of Protein Structure and Function

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