



Protein Dynamics, Function, and Design

Edited by
Oleg Jardetzky and
Jean-François Lefèvre

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Protein Dynamics Function And Design

Yicheng Fang



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 macromolecular 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 Protein/DNA Complexes by NMR Angela M Gronenborn 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 37 Andreas Plückthun 5 High Pressure Effects on Protein Structure

Understanding Protein Dynamics, Binding and Allostery for Drug Design Guang Hu, Pemra Doruker, Hongchun Li, Ebru Demet Akten, 2021-06-08 **Evolution, Origin of Life, Concepts and Methods** Pierre Pontarotti, 2019-10-01 This book presents 15 selected contributions to the 22nd Evolutionary Biology Meeting which took place in September 2018 in Marseille They are grouped under the following major themes Origin of Life Concepts and Methods Genome and Phenotype Evolution The aims of these annual meetings in Marseille are to bring together leading evolutionary biologists and other scientists who employ evolutionary biology concepts e.g. for medical research and to promote the exchange of ideas and encourage interdisciplinary collaborations Offering an up to date overview of recent advances in the field of evolutionary biology this book represents an invaluable source of information for scientists teachers and advanced students Invitation to Protein Sequence Analysis Through Probability and Information Daniel 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 Structural Biology in Drug Discovery Jean-Paul

Renaud,2020-02-05 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 allosteric 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 Biomedical Index to PHS-supported Research ,1991

Cumulated Index to the Books ,1999 From 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

Structures and Mechanisms William N. Lipscomb,2002 This volume encompasses a wide range of chemistry with juxtaposition of for example boron hydrides quantum mechanical calculations and structure of a virus providing a perspective

on chemistry not offered by traditional texts The breadth of this book will be stimulating and cause readers to think a little beyond the usual confines of a particular research field The book begins with an autobiographical reflection by Lipscomb and includes an introduction to the science of William N Lipscomb This volume encompasses a wide range of chemistry with a juxtaposition of for example boron hydrides quantum mechanical calculations and structure of a virus providing a perspective on chemistry not offered by traditional texts The volume includes chapters on polyhedral boranes oscillations waves and patterns in chemistry and biology interference of atom lasers chemical theory of bonding and NMR parameters NMR and EPR of proteins biological energy transduction protein ligand interactions and relation of structures to the central dogma of biology and concludes with comments on the relation of the retrovirus core to the function of this molecular machine

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Concepts in Protein Engineering and Design Paul Wrede,Gisbert Schneider,1994 No detailed description available for Concepts in Protein Engineering and Design *Science* John Michels (Journalist),2010 *The Cumulative Book Index* ,1999 **Dissertation Abstracts International** ,2006 *American Book Publishing Record* ,1999 **Graduate Programs in Physics, Astronomy and Related Fields** American Institute of Physics,2001 Philosophical Transactions ,2006 Each issue of Transactions B is devoted to a specific area of the biological sciences including clinical science All papers are peer reviewed and edited to the highest standards Published on the 29th of each month Transactions B is essential reading for all biologists

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