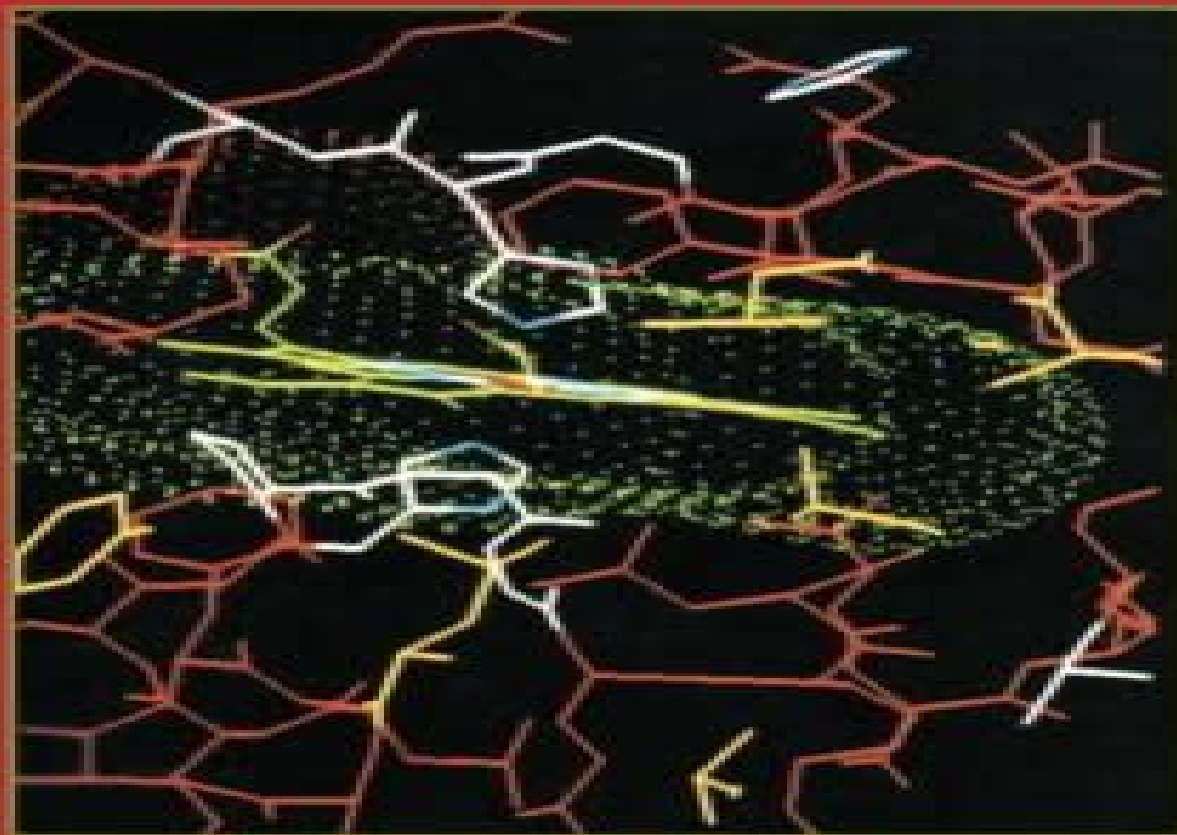


Crystallography Made Crystal Clear

A Guide for Users of
Macromolecular Models



Gale Rhodes

Crystallography Made Crystal Clear Third Edition A For S Of Macromolecular Models Complementary Science

Gale Rhodes



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Improved Methods for Characterization of Protein Dynamics by NMR

spectroscopy and Studies of the EphB2 Kinase Domain Alexandra Ahlner, 2015-04-15 Proteins are essential for all known forms of life and in many lethal diseases protein failure is the cause of the disease To understand proteins and the processes they are involved in it is valuable to know their structures as well as their dynamics and interactions The structures may not be directly inspected because proteins are too small to be visible in a light microscope which is why indirect methods such as nuclear magnetic resonance NMR spectroscopy have to be utilized This method provides atomic information about the protein and in contrast to other methods with similar resolution the measurements are performed in solution resulting in more physiological conditions enabling analysis of dynamics Important dynamical processes are the ones on the millisecond timeframe which may contribute to interactions of proteins and their catalysis of chemical reactions both of significant value for the function of the proteins To better understand proteins not only do we need to study them but also develop the methods we are using This thesis presents four papers about improved NMR techniques as well as a fifth where the kinase domain of ephrinB receptor 2 EphB2 has been studied regarding the importance of millisecond dynamics and interactions for the activation process The first paper presents the software COMPASS which combines statistics and the calculation power of a computer with the flexibility and experience of the user to facilitate and speed up the process of assigning NMR signals to the atoms in the protein The computer program PINT has been developed for easier and faster evaluation of NMR experiments such as those that evaluate protein dynamics It is especially helpful for NMR signals that are difficult to distinguish so called overlapped peaks and the soft ware also converts the detected signals to the indirectly measured physical quantities such as relaxation rate constants principal for dynamics Next are two new versions of the Carr Purcell Maiboom Gill CPMG dispersion pulse sequences designed to measure millisecond dynamics in a way so that the signals are more separated than in standard experiments to reduce problems with overlaps To speed up the collection time of the data set a subset is collected and the entire data set is then reconstructed by multi dimensional decomposition co processing Described in the thesis is also a way to produce suitably labeled proteins to detect millisecond dynamics at C positions in proteins using the CPMG dispersion relaxation experiment at lower protein concentrations Lastly the kinase domain of EphB2 is shown to be more dynamic on the millisecond time scale as well as more prone to interact with itself in the active form than in the inactive one This is important for the receptor function of the protein when and how it mediates signals To conclude this work has extended the possibilities to study protein dynamics by NMR spectroscopy and contributed to increased understanding of the activation process of EphB2 and its signaling mechanism *The British National*

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tutorials in molecular modeling on personal computers Crystallography Made Crystal Clear Arwen R. Pearson, Nicholas Pearce, Jennifer Wierman, 2022-01-15 Crystallography Made Crystal Clear makes crystallography accessible to readers who have no prior knowledge of the field or its mathematical basis It provides a comprehensive and concise reference for beginning macromolecular crystallographers and non specialist users of crystallographic models Visual and geometric models are used to help readers understand the physics and mathematics that form the basis of X ray crystallography and to understand both the extent but also limitations of the information that can be obtained in a diffraction experiment Importantly readers will learn how to use modern web based tools to evaluate model and data quality This updated and expanded new edition also includes discussion of the recent advances in infrastructure and automation and how these have impacted structural biology Uses accessible language and updated graphics to explain complex topics Covers both traditional single crystal data collection as well as serial data collection and long wavelength crystallography the unique aspects of which are not currently covered in any other text Includes new chapters describing model building and model validation procedures with step by step guidance **Introduction to Macromolecular Crystallography** Alexander McPherson, 2011-09-20 A comprehensive and approachable introduction to crystallography now updated in a valuable new edition The Second Edition of this well received book continues to offer the most concise authoritative and easy to follow introduction to the field of crystallography Dedicated to providing a complete basic presentation of the subject that does not assume a background in physics or math the book s content flows logically from basic principles to methods such as those for solving phase problems interpretation of Patterson maps and the difference Fourier method the fundamental theory of diffraction and the properties of crystals and applications in determining macromolecular structure This new edition includes a vast amount of carefully updated materials as well as two completely new chapters on recording and compiling X ray data and growing crystals of proteins and other macromolecules Richly illustrated throughout to clarify difficult concepts this book takes a non technical approach to crystallography that is ideal for professionals and graduate students in structural biology biophysics biochemistry and molecular biology who are studying the subject for the first time **Macromolecular Crystallography** Mark R. Sanderson, Jane V. Skelly, 2007-08-23 Macromolecular Crystallography is the study of macromolecules proteins and nucleic acids using X ray crystallographic techniques in order to determine their molecular structure The knowledge of accurate molecular structures is a pre requisite for rational drug design and for structure based function studies to aid the development of effective therapeutic agents and drugs The successful determination of the complete genome genetic sequence of several species including humans has recently directed scientific attention towards identifying the structure and function of the complete complement of proteins that make up that species a new and rapidly growing field of study called structural genomics There are now several important and well funded global initiatives in operation to identify all of the proteins of key model species One of the main requirements for these initiatives is a high

throughput crystallization facility to speed up the protein identification process The extent to which these technologies have advanced calls for an updated review of current crystallographic theory and practice This practical reference book features the latest conventional and high throughput methods and includes contributions from a team of internationally recognized leaders and experts It will be of relevance and use to graduate students research scientists and professionals currently working in the field of conventional and high throughput macromolecular crystallography **Macromolecular**

Crystallography, Part D Charles W. Carter Jr., Charles W. Carter, Robert M. Sweet, 2003-12-10 Accurate molecular structures is vital for rational drug design and for structure based functional studies directed toward the development of effective therapeutic agents and drugs Crystallography can reliably predict structure both in terms of folding and atomic details of bonding Phases Map interpretation and refinement Analysis and software Macromolecular Crystallography, Part C Charles W. Carter Jr., 2003-12-15 Accurate molecular structures are vital for rational drug design and for structure based functional studies directed toward the development of effective therapeutic agents and drugs Crystallography can reliably predict structure both in terms of folding and atomic details of bonding Methodological methods in crystals Methodological methods data analysis Macromolecular Crystallography Charles W. Carter, Robert M. Sweet, 2003

Macromolecular Crystallization and Crystal Perfection Naomi E Chayen, John R Helliwell, Edward H Snell, 2010-03-25 Structural biology is key to our understanding of the mechanisms of biological processes This book describes current methods and future frontiers in crystal growth and use of X ray and Neutron crystallography in the context of the very successful current automation of crystallization and generation of synchrotron X ray and neutron beams

Macromolecular Physics Bernhard Wunderlich, 1980-07 This third volume completes the first part of the project Macromolecular Physics The first volume dealt with the description of macromolecular crystals the second volume dealt with crystal growth and the third volume summarizes our knowledge of the melting of linear flexible macromolecules The discussion in the three volumes goes from reasonably well established topics such as the structure morphology and defects in crystals to topics still in flux such as crystal nucleation detailed growth mechanisms and annealing processes to arrive at the present topics of equilibrium nonequilibrium and copolymer melting Our knowledge is quite limited on many aspects of these latter topics Macromolecular Crystallography Maria Armenia Carrondo, Paola Spadon, 2011-12-01 This volume is a collection of the contributions presented at the 42nd Erice Crystallographic Course whose main objective was to train the younger generation on advanced methods and techniques for examining structural and dynamic aspects of biological macromolecules The papers review the techniques used to study protein assemblies and their dynamics including X ray diffraction and scattering electron cryo electron microscopy electro nanospray mass spectrometry NMR protein docking and molecular dynamics A key theme throughout the book is the dependence of modern structural science on multiple experimental and computational techniques and it is the development of these techniques and their integration that will take

us forward in the future **Macromolecular Crystallography Protocols, Volume 1** Sylvie Doublié, 2010-11-10

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