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Very Important Paper

Protein-Protein Recognition Involved in the Intermodular Transacylation Reaction in Modular Polyketide Synthase in the Biosynthesis of Vicenistatin

Taichi Chisuga,[a] Akimasa Miyanaga,*[a] and Tadashi Eguchi*[a]

The ketosynthase (KS) domain is a core domain found in modular polyketide synthases (PKSs). To maintain the polyketide biosynthetic fidelity, the KS domain must only accept an acyl group from the acyl carrier protein (ACP) domain of the immediate upstream module even when they are separated into different polypeptides. Although it was reported that both the docking domain-based interactions and KS-ACP compatibility are important for the interpolypeptide transacylation reaction in 6-deoxyerythronolide B synthase, it is not clear whether these findings are broadly applied to other modular PKSs. Herein, we describe the importance of protein-protein recognition in the intermodular transacylation between VinP1 module 3 and VinP2 module 4 in vicenistatin biosynthesis. We compared the transacylation activity and crosslinking efficiency of VinP2 KS_4 against the cognate VinP1 ACP_3 with the non-cognate one. As a result, it appeared that VinP2 KS_4 distinguishes the cognate ACP_3 from other ACPs.

Introduction

Polyketide synthases (PKSs) are responsible for the biosynthesis of various structurally diverse bioactive polyketide natural products.[1] Bacterial modular type I PKSs are huge multifunctional proteins, and are comprised of multiple modules, each of which contains a set of catalytic domains for one round of polyketide chain elongation.[2] Ketosynthase (KS), acyltransferase (AT), and acyl carrier protein (ACP) domains are essential for the polyketide chain elongation in each module. In the polyketide chain elongation in the Nth module, the AT domain (AT_N) transfers a specific malonyl-type extender unit onto the terminal thiol group of the phosphopantetheine arm of the ACP_N. KS_N receives the growing polyketide chain on the thiol group of the catalytic Cys residue from the ACP domain (ACP_{N-1}) of the upstream N-1th module, and subsequently catalyzes a decarboxylative Claisen-like condensation with the malonyl-type extender unit on ACP_N to afford β-ketoacyl-ACP_N (Figure 1). This β-ketoacyl-group is optionally modified by reduction and dehydration reactions catalyzed by other catalytic domains thus completing the polyketide chain elongation in the Nth module. The acyl group on ACP_N is transferred to KS_{N+1}, which initiates the polyketide chain elongation in the N+1th module. To maintain the structural integrity of the polyketide products, the growing polyketide chain must be transferred between modules in the correct order.

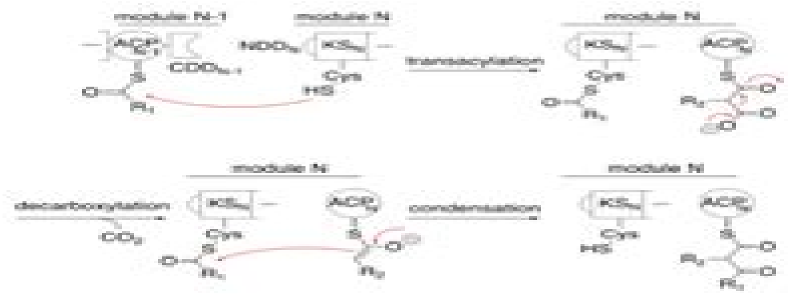

Figure 1. Proposed reaction mechanism of the type I PKS KS domain.

For the functional intermodular transacylation reaction of the KS_N domain, KS_N must only accept an acyl group from the ACP_{N-1} domain of the immediate upstream module. When KS_N and ACP_{N-1} are separated into different polypeptides, complementary short linker regions referred to as docking domains (DDs) located at the N-terminus of KS_N and C-terminus of ACP_{N-1} (called NDD_N and CDD_{N-1}, respectively) have been shown to mediate the functional intermodular transacylation reaction between polypeptides.[3] Several studies show that docking domain compatibility is essential to maintain the biosynthetic fidelity in the intermodular transacylation reaction between polypeptides in bacterial *cis*-AT PKSs.[4–7] The protein-protein recognition between KS_N and ACP_{N-1} was also reported to be important in the intermodular transacylation reaction between polypeptides in 6-deoxyerythronolide B synthase (DEBS).[8,9] However, studies on the KS_N-ACP_{N-1} interactions between

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Protein Protein Recognition

Jacqueline M. Matthews

Protein Protein Recognition:

Protein-protein Recognition Colin Kleanthous,2000 The purpose of Protein Protein Recognition is to bring together concepts and systems pertaining to protein protein interactions in a single unifying volume In the light of the information from the genome sequencing projects and the increase in structural information it is an opportune time to try to make generalizations about how and why proteins form complexes with each other The emphasis of the book is on heteromeric complexes complexes in which each of the components can exist in an unbound state and will use well studied model systems to explain the processes of forming complexes After an introductory section on the kinetics thermodynamics analysis and classification of protein protein interactions weak intermediate and high affinity complexes are dealt with in turn Weak affinity complexes are represented by electron transfer proteins and integrin complexes Anti lysozyme antibodies the MHC proteins and their interactions with T cell receptors and the protein interactions of eukaryotic signal transduction are the systems used to explain complexes with intermediate affinities Finally tight binding complexes are represented by the interaction of protein inhibitors with serine proteases and by nuclease inhibitor complexes Throughout the chapters common themes are the technologies which have had the greatest impact how specificity is determined how complexes are stabilized and medical and industrial applications *Structure-driven Approaches to Protein-protein Recognition* Julian Mintseris,2006 Abstract Much of our understanding of protein function arises from the cellular context in which the protein operates While two proteins may be functionally linked in a variety of ways the most direct way for them to interact is through physical recognition of the protein surface followed by a binding event If the function of a single protein can be understood in terms of its interactions then the function of a biological system as a whole can be viewed through the network of protein interactions I use structure driven approaches to gain additional insight into the organization of protein interaction networks by showing distinct differences between transient and obligate protein interactions This important distinction can be detected on a purely structural level by comparing the pair wise contact frequencies between different types of atoms at the protein complex interface On the functional level the distinction can be made by looking at the curated ontology annotations Proteins involved in transient and obligate interactions have been subject to different levels of evolutionary pressure and traces of these differences can be detected by considering their evolutionary histories Residues in the interfaces of obligate complexes tend to evolve at a relatively slower rate allowing them to co evolve with their interacting partners In contrast the plasticity inherent in transient interactions leads to an increased rate of substitution for the interface residues and leaves little or no evidence of correlated mutations Recent advances in high throughput proteomic technologies combined with computational approaches have identified large numbers of putative novel interactions However both experimental and computational approaches tend to do better identifying components of large obligate complexes while fleeting interactions crucial in systems such as signaling cascades and immune response are harder to predict To this end I developed new representations of protein structure and derived empirical potentials for protein protein docking improving on our ability to predict the complex structures of transient complexes from individually crystallized components Protein-protein Recognition and Electron Transfer Ekaterina Vadimovna Pletneva,2001 Electron transfer ET between redox proteins plays an important role in many biological processes The first stage in the interprotein ET involves specific recognition and binding of protein molecules We are studying several diprotein systems to better understand the rules of protein protein recognition and conformational interconversion that might control the ET process To explore interactions between azurin and cytochrome c we investigated the effects of ionic strength on the kinetics of photoinduced ET reactions of the triplet state of zinc substituted cytochrome c 3Zncyt with the wild type and the following mutants of azurin Met44Lys Met64Glu and the double mutant Met44Lys Met64Glu Mutations in the hydrophobic patch of azurin significantly affect the reactivity of the protein with 3Zncyt Both kinetic effects of mutation and analysis of dipolar interactions indicated the involvement of the hydrophobic patch of azurin in the reaction In the study of a new plastocyanin from fern we used cytochrome c to explore the surface of the new protein and to learn about its ET properties At low ionic strength at least three exponentials are needed to describe the quenching of 3Zncyt by fern cupriplastocyanin *Analysis and Prediction of Protein-protein Recognition* Matthew James Betts,1999 **Protein-protein Recognition** Ye Che,2003 Protein-protein Recognition Vladimir Potapov,2006

Analysis and Prediction of Side-chain Flexibility in Protein-protein Recognition Kevin Wiehe,2008 Abstract Protein protein interaction is an essential mechanism in biological systems It is fundamental to such diverse processes as the immunological response signaling cascades and the function of enzymes Understanding how proteins recognize and associate with each other has been a goal of biological research for decades Currently computational modeling of protein protein interactions has become a common tool in the attempt to understand molecular recognition Specifically protein protein docking algorithms which seek to predict the complexed protein structure from its unbound components have advanced rapidly in recent years Most of the progress in protein docking algorithms has come from the employment of a rigid body approximation of the unbound proteins in order to reduce the complexity of the problem Our own lab has demonstrated consistent success with such an approach utilizing our docking algorithm ZDOCK in the Critical Assessment of Protein Interactions CAPRI an international blind docking test Recently docking algorithms have begun to incorporate flexible proteins by modeling side chain conformational change Current attempts to predict side chain rearrangement upon complexation do so using a brute force methodology in which all interface residues are searched Such an approach is computationally intensive and may be unnecessarily inaccurate because of the blind nature of the search In order to address these flaws we have created and analyzed a protein protein docking benchmark dataset to discover the characteristics of side chains that can best estimate the likelihood of a residue to exhibit conformational change Our analysis shows that the majority of sidechains in the interface of protein complexes do not change position between the unbound and bound conformations Additionally the frequency of side chain conformational change in interface residues is only slightly higher than other protein surface residues Because of this small difference and the usually limited knowledge of the location of the interface prior to docking we developed a support vector machine SVM approach that allows us to apply a probability of flexibility for all surface residues Here we describe the accuracy of this predictive method and its potential for application to protein protein docking **Protein-protein Recognition in the Complex Formed Between Cytochrome C Peroxidase and Cytochrome C** Qipan Zhang,1991 Computational Protein-Protein Interactions Ruth Nussinov,Gideon Schreiber,2009-06-26 Often considered the workhorse of the cellular machinery proteins are responsible for functions ranging from molecular motors to signaling The broad recognition of their involvement in all cellular processes has led to focused efforts to predict their functions from sequences and if available from their structures An overview of current resear

Computational Knowledge-based Prediction of Protein-protein Recognition Dennis Manfred Krüger,2014

Nucleic Acid–Protein Recognition Henry Vogel,2012-12-02 Nucleic Acid Protein Recognition covers the proceedings of a symposium on Nucleic Acid Protein Recognition held at Arden House Harriman Campus of Columbia University on May 30 June 1 1976 The symposium inaugurated the P S Biomedical Sciences Symposia under the sponsorship of the College of Physicians and Surgeons of Columbia University This book is organized into nine part encompassing 31 chapters The opening parts describe the principles of DNA replication and the unique chromatin structure These parts also examine the physical chemistry of the interactions of melting proteins with nucleic acids The third part presents the different types of approaches that can be used to study the function of RNA polymerases and the development of a cell free system that favors Pol II catalyzed transcription from type 2 adenovirus DNA Parts IV and V deal with the sequence determination of wild type and mutant repressor and the restriction and modification of DNA endonucleases while parts VI and VII focus of the recognition of tRNA Part VIII discusses some significant studies on the assembly of ribosomes and the principles of ribosomal interactions Lastly Part IX considers the role of small RNA template in the reaction mechanism of RNA replicases and ribonucleases This part also surveys the so called RNase III cleavage of different types of RNA and the structure of nucleic acid protein complexes Protein Surface Recognition Ernest Giralt,Mark Peczuh,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 **Proteomics and Protein-Protein Interactions** Gabriel Waksman,2006-12-22 Gabriel Waksman Institute of Structural Molecular Biology Birkbeck and University College London Malet Street London WC1E 7HX United Kingdom Address for correspondence Professor Gabriel Waksman Institute of Structural Molecular Biology Birkbeck and University College London Malet Street London WC1E 7H United Kingdom Email g waksman bbk ac uk and g waksman ucl ac uk Phone 44 0 207 631 6833 Fax 44 0 207 631 6833 URL http people cryst bbk ac uk ubcg54a Gabriel Waksman is Professor of Structural Molecular Biology at the Institute of Structural Molecular Biology at UCL Birkbeck of which he is also the director Before joining the faculty of UCL and Birkbeck he was the Roy and Diana Vagelos Professor of Biochemistry and Molecular Biophysics at the Washington University School of Medicine in St Louis USA The rapidly evolving eld of protein science has now come to realize the ubiquity and importance of protein protein interactions It had been known for some time that proteins may interact with each other to form functional complexes but it was thought to be the property of only a handful of key proteins However with the advent of hi throughput proteomics to monitor protein protein interactions at an organism level we can now safely state that protein protein interactions are the norm and not the exception **Protein Modules and Protein-Protein Interactions** ,2002-11-24 Protein modules engage in a multitude of interactions with one another and with other cellular components notably with DNA These interactions are a central aspect of protein function of great relevance in the post genomic era This volume describes a panel of approaches for analyzing protein modules and their interactions ranging from bioinformatics to physical chemistry to biochemistry with an emphasis on the structure function relationship in protein protein complexes involved in cellular processes including signal transduction Comprehensive overview of different facets of macromolecule interactions Computational and bioinformatics aspects of analyzing protein modules and their interactions Emphasis on structure function relationship in protein protein complexes involved in cellular processes

Protein-Protein Interactions Michael D. Wendt,2012-06-26 Michael D Wendt Protein Protein Interactions as Drug Targets Shaomeng Wang Yujun Zhao Denzil Bernard Angelo Aguilar Sanjeev Kumar Targeting the MDM2 p53 Protein Protein Interaction for New Cancer Therapeutics Kurt Deshayes Jeremy Murray Domagoj Vucic The Development of Small Molecule IAP Antagonists for the Treatment of Cancer John F Kadow David R Langley Nicholas A Meanwell Michael A Walker Kap Sun Yeung Richard Pracitto Protein Protein Interaction Targets to Inhibit HIV 1 Infection Nicholas A Meanwell David R Langley Inhibitors of Protein Protein Interactions in Paramyxovirus Fusion a Focus on Respiratory Syncytial Virus Andrew B Mahon

Stephen E Miller Stephen T Joy Paramjit S Arora Rational Design Strategies for Developing Synthetic Inhibitors of Helical Protein Interfaces Michael D Wendt The Discovery of Navitoclax a Bcl 2 Family Inhibitor **Computational Knowledge-Based Prediction of Protein-Protein Recognition** Dennis M. Krüger,2014 **Protein-Protein Docking** Agnieszka A. Kaczor,2024-07-10 This volume covers a wide array of topics on protein protein docking ranging from the fundamentals of the method and its recent developments to docking tools and examples of protein protein docking applications The chapters in this book are organized into four parts Part One looks at the fundamentals of protein protein docking such as rigid and flexible docking and sampling and scoring in protein protein docking Part Two focuses on the latest advancements made in the field such as how the protein backbone flexibility is treated Part Three explores practical applications of protein protein docking tools and databases with emphasis on software for predicting binding free energy of protein protein complexes and their mutants Part Four talks about protein protein docking approaches to different systems and their challenges and strategies of molecular docking of intrinsically disordered proteins Written in the highly successful Methods in Molecular Biology series format chapters include introductions to their respective topics lists of the necessary materials and reagents step by step readily reproducible laboratory protocols and tips on troubleshooting and avoiding known pitfalls Cutting edge and thorough Protein Protein Docking Methods and Protocols is a valuable resource for structural biologists bioinformaticians molecular modelers and medicinal chemists looking to learn more about this important field **Protein'Protein Interactions** Haian Fu,2008-02-03 As the mysteries stored in our DNA have been more completely revealed scientists have begun to face the extraordinary challenge of unraveling the int cate network of protein protein interactions established by that DNA fra work It is increasingly clear that proteins continuously interact with one another in a highly regulated fashion to determine cell fate such as proliferation diff entiation or death These protein protein interactions enable and exert str gent control over DNA replication RNA transcription protein translation macromolecular assembly and degradation and signal transduction essentially all cellular functions involve protein protein interactions Thus protein p tein interactions are fundamental for normal physiology in all organisms Alt ation of critical protein protein interactions is thought to be involved in the development of many diseases such as neurodegenerative disorders cancers and infectious diseases Therefore examination of when and how protein p tein interactions occur and how they are controlled is essential for understa ing diverse biological processes as well as for elucidating the molecular basis of diseases and identifying potential targets for therapeutic interventions Over the years many innovative biochemical biophysical genetic and computational approaches have been developed to detect and analyze p tein protein interactions This multitude of techniques is mandated by the diversity of physical and chemical properties of proteins and the sensitivity of protein protein interactions to cellular conditions **Protein-Protein Interactions** Krishna Mohan Poluri,Khushboo Gulati,Sharanya Sarkar,2021-05-19 This book provides a comprehensive overview of the fundamental aspects of protein protein interactions PPI including a detailed account of the energetics and thermodynamics involved in these interactions It also discusses a number of computational and experimental approaches for the prediction of PPI interactions and reviews their principles advantages drawbacks and the recent developments Further it offers structural and mechanistic insights into the formation of protein protein complexes and maps different PPIs into networks to delineate various pathways that operate at the cellular level Lastly it describes computational protein protein docking techniques and discusses their implications for further experimental research Given its scope this book is a valuable resource for students researchers scientists entrepreneurs and medical healthcare professionals *Protein Dimerization and Oligomerization in Biology* Jacqueline M. Matthews,2012-09-04 This volume has a strong focus on homo oligomerization which is surprisingly common However protein function is so often linked to both homo and hetero oligomerization and many heterologous interactions likely evolved from homologous interaction so this volume also covers many aspects of hetero oligomerization

Protein Protein Recognition Book Review: Unveiling the Power of Words

In a world driven by information and connectivity, the energy of words has become more evident than ever. They have the capacity to inspire, provoke, and ignite change. Such is the essence of the book **Protein Protein Recognition**, a literary masterpiece that delves deep into the significance of words and their impact on our lives. Written by a renowned author, this captivating work takes readers on a transformative journey, unraveling the secrets and potential behind every word. In this review, we will explore the book is key themes, examine its writing style, and analyze its overall effect on readers.

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Protein Protein Recognition Introduction

In todays digital age, the availability of Protein Protein Recognition books and manuals for download has revolutionized the way we access information. Gone are the days of physically flipping through pages and carrying heavy textbooks or manuals. With just a few clicks, we can now access a wealth of knowledge from the comfort of our own homes or on the go. This article will explore the advantages of Protein Protein Recognition books and manuals for download, along with some popular platforms that offer these resources. One of the significant advantages of Protein Protein Recognition books and manuals for download is the cost-saving aspect. Traditional books and manuals can be costly, especially if you need to purchase several of them for educational or professional purposes. By accessing Protein Protein Recognition versions, you eliminate the need to spend money on physical copies. This not only saves you money but also reduces the environmental impact associated with book production and transportation. Furthermore, Protein Protein Recognition books and manuals for download are incredibly convenient. With just a computer or smartphone and an internet connection, you can access a vast library of resources on any subject imaginable. Whether youre a student looking for textbooks, a professional seeking industry-specific manuals, or someone interested in self-improvement, these digital resources provide an efficient and accessible means of acquiring knowledge. Moreover, PDF books and manuals offer a range of benefits compared to other digital formats. PDF files are designed to retain their formatting regardless of the device used to open them. This ensures that the content appears exactly as intended by the author, with no loss of formatting or missing graphics. Additionally, PDF files can be easily annotated, bookmarked, and searched for specific terms, making them highly practical for studying or referencing. When it comes to accessing Protein Protein Recognition books and manuals, several platforms offer an extensive collection of resources. One such platform is Project Gutenberg, a nonprofit organization that provides over 60,000 free eBooks. These books are primarily in the public domain, meaning they can be freely distributed and downloaded. Project Gutenberg offers a wide range of classic literature, making it an excellent resource for literature enthusiasts. Another popular platform for Protein Protein Recognition books and manuals is Open Library. Open Library is an initiative of the Internet Archive, a non-profit organization dedicated to digitizing cultural artifacts and making them accessible to the public. Open Library hosts millions of books, including both public domain works and contemporary titles. It also allows users to borrow digital copies of certain books for a limited period, similar to a library lending system. Additionally, many universities and educational institutions have their own digital libraries that provide free access to PDF books and manuals. These libraries often offer academic texts, research papers, and technical manuals, making them invaluable resources for students and researchers. Some notable examples include MIT OpenCourseWare, which offers free access to course materials from the Massachusetts Institute of Technology, and the Digital Public Library of America, which provides a vast collection of digitized books and historical documents. In conclusion, Protein Protein Recognition books and manuals for download have transformed the way we access information. They provide a cost-effective and convenient means of acquiring knowledge, offering the ability to access a vast library of resources at our fingertips. With platforms like Project Gutenberg, Open Library, and various digital libraries offered by educational institutions, we have access to an ever-expanding collection of books and manuals. Whether for educational, professional, or personal purposes, these digital resources serve as valuable tools for continuous learning and self-improvement. So why not take advantage of the vast world of Protein Protein Recognition books and manuals for download and embark on your journey of knowledge?

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