

Protein Structure And Evolution: Papers And Discussion

Heredity (2007), 1–13
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SHORT REVIEW

The quest for natural selection in the age of comparative genomics

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Continued genome sequencing has fueled progress in statistical methods for understanding the action of natural selection at the molecular level. This article reviews various statistical techniques (and their applicability) for detecting adaptation events and the functional divergence of proteins. As large-scale automated studies become more frequent, they provide a useful resource for generating biological null hypotheses for further experimental and statistical testing. Furthermore, they shed light on typical patterns of lineage-specific evolution of organisms, on the functional and

structural evolution of protein families and on the interplay between the two. More complex models are being developed to better reflect the underlying biological and chemical processes and to complement simpler statistical models. Linking molecular processes to their statistical signatures in genomes can be demanding, and the proper application of statistical models is discussed. *Heredity* advance online publication, 12 September 2007; doi:10.1038/sj.hdy.6801052

Keywords: functional divergence; positive selection; comparative genomics; molecular evolution; protein structure; population genetics

Introduction

Genomic change underlies the biodiversity found on Earth. Rapid genome sequencing coupled with the development of statistical methods for comparative genomics has enabled the examination of forces driving lineage-specific divergence at the molecular level. In an early study focusing on a comparison of human and chimpanzee, the 'lineage' divergence suggested the hypothesis that evolutionary changes in gene regulation have driven phenotypic divergence between species (King and Wilson, 1975). More recently, the rewiring of a regulatory pathway from the last common ancestor of the sea urchin and starfish toward both extant species (Hinman *et al.*, 2003) and the evolution of pigmentation in *Drosophila* (Prud'homme *et al.*, 2006) gave further support to this view. Although changes in coding sequences can be compensatory (Haag, 2007), changes at the protein-coding level clearly also play a vital role in phenotypic divergence, as experimental evidence of lineage-specific functional change of proteins has been found in a growing number of cases (Benner *et al.*, 2007). Detecting genes targeted by selection in the genome became an efficient strategy for finding causes of species differences and identifying genomic regions of functional, and potentially medical, significance. Rather than focus on the controversy surrounding the genomic basis of phenotypic evolution, we will assume that evolution of protein-coding

sequences contributes to changes in the phenotype and fitness of the organism and proceed with a discussion of computational methods to detect selection-driven changes leading to changes in molecular phenotype (protein function).

Several views exist of how gene sequence maps to protein function. From a gradualist viewpoint, proteins accumulate substitutions and this gradual change corresponds to a steady evolution of protein function. This is largely consistent with a neutralist view of protein evolution, in which functional change is not being driven by positive selection and is due to a random accumulation of mutations, but this scenario is now commonly incorporated into a selectionist viewpoint. With bursts of lineage-specific positive selection, punctuated periods of rapid sequence change may occur on a few branches (Gould and Eldredge, 1993), whereas negative selection and functional stasis are seen on others (Messier and Stewart, 1997). Both gradualist and punctuated views of protein sequence evolution are consistent with protein structure dictating sites where substitution can occur and those where any change would radically diminish protein fitness, on the basis of both binding interactions and folding constraints (Bloom *et al.*, 2007; Lin *et al.*, 2007). Functionally important sites are expected to evolve slowly, whereas rapid changes are expected at sites that have little impact on the structure and function of the protein (neutral positions) or at sites where diversification is favored through increased fitness of the organism or necessitated as compensatory changes (Depristo *et al.*, 2005; Lin *et al.*, 2007). Such heterogeneity across sites is frequently modeled with a γ distribution (Yang, 1996; Stern and Pupko, 2006). Changes to protein function can be altered not just by changes in specific amino acids

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Received 30 April 2007; revised 19 June 2007; accepted 3 August 2007

Protein structure and evolution: [papers and discussion [Czechoslovakia) (Fox, Jack Lawrence, ; Deyl, ZdenTek. ; BlaTzej, Anton. ; International Union of Protein structure and evolution: [papers and discussion. I.U.B. Symposium on Protein Structure and Evolution (Smolenice and Kocovce, Czechoslovakia).Protein structure and evolution: [papers and discussion / edited by] J. Lawrence Fox, Author: I.U.B. Symposium on Protein Structure and Evolution (The assignment described here, one that investigates protein structure and . Attention also was paid to selecting papers that discussed proteins across a range of contexts (e.g., ecological, medical, evolutionary, molecular, biochemical) .protein. We also discuss the constraints protein complex structures impose on sequence integrate residue evolution, structure evolution, and to quantify Papers of particular interest, published within the period of review.Purchase The Evolution of Protein Structure and Function - 1st Edition. The papers presented by Emil's colleagues, friends, and students from all phases of his long and varied scientific career provided a valuable Discussion and Summary.In this paper we focus on protein interaction networks, whose nodes correspond to . We note that in our discussion of node dynamics we have not separately.In this paper, we describe in outline the structural changes that occur during evolution and discuss how their nature and extent are determined by the intrinsic .In this paper we ask whether we can infer evolutionary constraints from a is analogous to protein structure prediction reports that discuss the.paper we present a new optimization approach using the Index Terms Protein, Differential Evolution, Structural class . RESULTS AND DISCUSSION.Large-scale studies of protein structure evolution can begin The analysis presented in this paper was compiled on the basis of the largest . Discussion.This paper discusses a number of methods to predict protein functional site especially . FREPS is discussed in sequence and structure based method section. .. is a protein ligand binding site prediction algorithm that integrates evolutionary.Starting from an initial seed lattice structure, evolution of model proteins progresses by sequence .. We are grateful to Eric Deeds and Richard Goldstein for useful discussions. This paper was submitted directly (Track II) to the PNAS office.Full-Text Paper (PDF): Bioinformatics Tools for Protein Analysis. The protein structure databases discussed in this paper are such as Protein Data Bank, NCBI Structure Database .. protein domain conserved during molecular evolution.What I want to address is why the problem of protein evolution is such a big The paper by Romero and Arnold that Poenie cites in support of claim #3 is with the same structure and function, but different amino acid sequences. novel protein-coding sequences (orphan genes discussed here) appear to.matrix, Protein structure alignment, Designability, Evolution, Contact order, Throughout the paper we suggest several discussions that are.Protein structure evolution. Papers. Structural Bridges through Fold Space There is also discussion about whether protein structure space could really be.annotating enzyme structures of unknown function and for designing novel . The Structure and Evolution of Enzymes. Discussion. .. Receptors and binding proteins analysed for bond length changes..

Paper I concerns how structures respond to evolutionary changes in protein methodology, a brief summary of results and a discussion of my contributions. In this paper we discuss the most important algorithms like evolutionary algorithms, particle swarm or ant colony optimization and computational methods. Conceptually, we will explore the problem of protein folding and protein Assigned Paper for Summary and Discussion (Gardner, Cell) Evolution of IDPs.

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