

Dictionary-driven protein annotation

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Received January 17, 2002; Revised and Accepted June 4, 2002

ABSTRACT

Computational methods seeking to automatically determine the properties (functional, structural, physicochemical, etc.) of a protein directly from the sequence have long been the focus of numerous research groups. With the advent of advanced sequencing methods and systems, the number of amino acid sequences that are being deposited in the public databases has been increasing steadily. This has in turn generated a renewed demand for automated approaches that can annotate individual sequences and complete genomes quickly, exhaustively and objectively. In this paper, we present one such approach that is centered around and exploits the Bio-Dictionary, a collection of amino acid patterns that completely covers the natural sequence space and can capture functional and structural signals that have been reused during evolution, within and across protein families. Our annotation approach also makes use of a weighted, position-specific scoring scheme that is unaffected by the over-representation of well-conserved proteins and protein fragments in the databases used. For a given query sequence, the method permits one to determine, in a single pass, the following: local and global similarities between the query and any protein already present in a public database; the likeness of the query to all available archaeal/bacterial/eukaryotic/viral sequences in the database as a function of amino acid position within the query; the character of secondary structure of the query as a function of amino acid position within the query; the cytoplasmic, transmembrane or extracellular behavior of the query; the nature and position of binding domains, active sites, post-translationally modified sites, signal peptides, etc. In terms of performance, the proposed method is exhaustive, objective and allows for the rapid annotation of individual sequences and full genomes. Annotation examples are presented and discussed in Results, including individual queries and complete genomes that were released publicly after we built the Bio-Dictionary that is used in our

experiments. Finally, we have computed the annotations of more than 70 complete genomes and made them available on the World Wide Web at <http://cbscrv.watson.ibm.com/Annotations/>.

INTRODUCTION

The automatic elucidation of protein function directly from sequence has been the focus of research activity for many years. Such an elucidation has an obvious appeal for it tries to minimize the amount of associated manual labor by reducing a large number of possibilities to one or a handful of choices. This is typically achieved by tapping into repositories of previously accumulated knowledge and by trading computation (i.e. *in silico* approaches) for typically tedious manual analysis. The discovery of protein function directly from sequence, in an automated or semi-automated manner, has become a fundamental question as thousands of unknown proteins and increasing numbers of complete genomes are made available daily in the public domain. Of course, one should not lose sight of the fact that protein annotation is the first step in the attempt to fully describe a particular organism through characterization of its metabolic pathways and transcription regulation networks.

During the last three decades, numerous methods have been proposed for determining protein function from sequence, all of which are essentially instances of a 'guilty by association' approach to solving this problem. Depending on the nature of the information exploited and the manner in which the information is used, these methods can essentially be divided into a handful of well-differentiated categories.

The chronologically earliest examples of protein annotation methods rely on the determination of a local or global similarity between a query protein and proteins with known annotation that are contained in a database (1–4). If two sequences of comparable length share a large portion of their extent, the previously uncharacterized sequence will inherit the function of the annotated one. The validity of this scheme relies on the implicit assumption that two sequences that 'look the same' at the sequence level also have the same function and structure. This is a reasonable assumption, but counter-examples such as the dehydrogenase/z-crystallin case have also been documented in the literature (for a discussion of this particular case see for example 5). The methods in this category are known as 'similarity-based' or 'homology-based' and are numerous. The approach we present in this paper belongs to this category as well.

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