

# Computing Closures of Indirect Similarity Relationships among Structures in Proteins

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## Abstract

*We have developed a deductive database system PACADE for analyzing three dimensional and secondary structures of protein. A function newly introduced to PACADE is described here. It enables to compute a closure of indirect similarity relationships among structure of proteins.*

## 1 Introduction

Because of the exponential increase of these *genome data*, there is a increasing need to develop a sound knowledge base to describe a hypothesis and to check it out with queries. We have developed a deductive database system PACADE for analyzing three dimensional and secondary structures of protein. By describing a set of declarative rules and giving a query to PACADE,

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a user can flexibly search for structures in proteins. As for the searches for super-secondary structures frequently found in proteins (e.g. Greek Keys and n-stranded meanders,) the deductive inference system of PACADE works well. To make PACADE an even more useful system for molecular biologists, we introduced a novel function which enables automatic searches for similar structures in proteins. Through this function, a user can search for structures of proteins similar to the one being examined.

However, to compute a closure of structures which includes a specific structure of a protein, it is insufficient and inefficient to use the similarity search function of PACADE, combinatorially. We describe here a function newly introduced into PACADE to resolve the problems. This function enables a non-combinatorial computation of a cluster of indirectly similar structures, which includes a specific structure given by a user in the form of a query.

## 2 Method and Result

Starting from a given structure in a specific protein, one can compute a closure of structures indirectly similar to it by regarding answers as closed queries and iterating direct similarity search in PACADE. Computation of closure is performed by fixpoint computation like the one in ordinary bottom-up evaluator. Thus, it can be optimized by using differential algorithm instead of naive algorithm. On the other hand, the constant bindings in closed queries are available to optimize through Magic Set transformation. A module, added to PACADE to perform closure computation, is implemented using these optimization techniques.

As the result of an example search starting from a specific structure (a0) in interleukin ("3i18"), we obtained a closure consisting of 6 structures (a0-a5). In Figure 1, bi-directional arrows represent direct similarity relationships among a0-a5. The graphical representations of a0-a5 reflect the fact that a2, a4 and a5 are similar (Figure 2.)

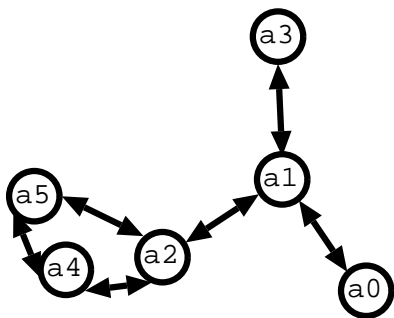


Figure 1: Similarity relationships among a0-a5

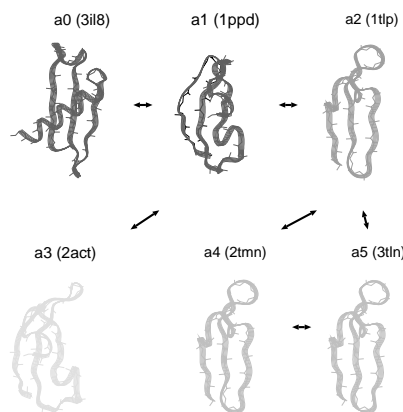


Figure 2: Graphical display of a0-a5

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