WebPACADE: A System for the Analysis of Structural Similarity of Protein via WWW

Kenji Satou [1]
ken@ims.u-tokyo.ac.jp

Toshihide Ono [2]
tosihide@grt.kyushu-u.ac.jp

Yukiko Nakanishi [2]
yukiko35@grt.kyushu-u.ac.jp

Emiko Furuichi [3]
emiko@fukuoka-wjc.ac.jp

Satoru Kuhara [2]
kuhara@grt.kyushu-u.ac.jp

Toshihisa Takagi [1]
takagi@ims.u-tokyo.ac.jp

[1] Human Genome Center, Institute of Medical Science, University of Tokyo
4-6-1 Shirokanedai, Minato-ku, Tokyo 108, Japan

[2] Graduate School of Genetic Resources Technology, Kyushu University
6-10-1 Hakozaki, Higashi-ku, Fukuoka 812, Japan

[3] Fukuoka Women's Junior College, 4-16-1 Gojo, Dazaifu, Fukuoka 818-01, Japan

Abstract

This paper describes on a developmental system WebPACADE which is an extended version of a deductive database system PACADE for the analysis of protein 3D structure. It enables structural similarity searches on various proteins in the level of secondary structure. Results of a similarity search can be displayed graphically in a WWW browser.

1 Introduction

Currently, Brookhaven's Protein Data Bank (PDB [1]) contains about five thousands of determined protein structures. However, no comprehensive tool for the retrieval of protein substructures based on their structural similarity has been brought into practical use. For that purpose, we have developed a deductive database system PACADE for analyzing three dimensional and secondary structures of protein [2]. Using deductive inference, it searches for similar substructures in proteins in the level of secondary structure [3]. To make PACADE more useful, we are equipping it with a WWW interface and a graphical view of retrieved protein substructures.

2 System

The new system, WebPACADE, consists of the following free softwares in addition to original data and programs.

- Coral deductive database system (`http://www.cs.wisc.edu/coral`)

- Chemscape Chime (`http://www.mdli.com/chemscape/chime/chime.html`)

- RasMol (`http://klaatu.oit.umass.edu/microbio/rasmol`)

Chime is a Netscape Navigator plug-in which is used to visualize results of structural similarity search by PACADE, while RasMol is used only for generating Chime scripts automatically. Before returning the results to a browser, the scripts are modified according to the results, that is, all substructures are unhighlighted except the answers of structural similarity search (Figure 1).
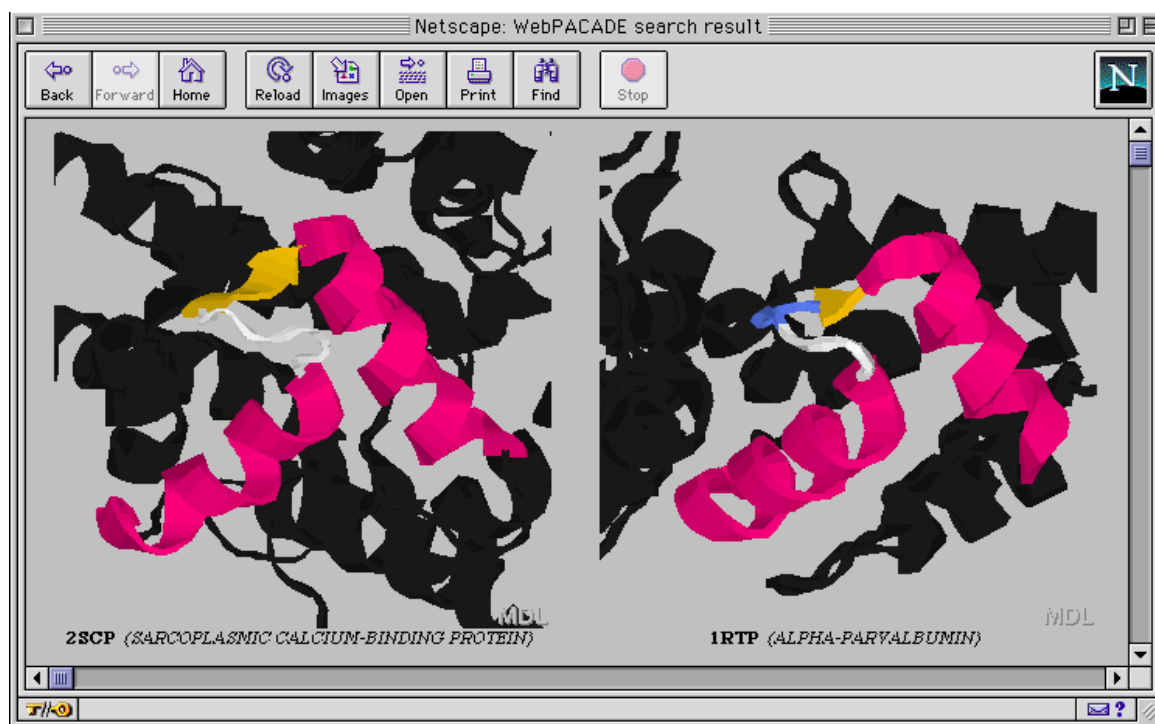
Figure 1: Screen shot of WebPACADE under development

3 Future Works

WebPACADE currently supports only 360 non-redundant structures in PDB. To support thousands of structures, the response of WebPACADE server, which runs on Solaris, should be improved by performance tuning and placing facts (persistent relations) in memory space.

Acknowledgments

References

[1] Bernstein, F. C., Koetzle, T. F., Williams, G. J. B., Meyer, E. F., Brice, M. D., Rodgers, J. R., Kennard, O., Shimanouchi, T. and Tasumi, M., *"The Protein Data Bank: A Computer-based Archival File for Macromolecular Structures"*, J. Mol. Biol., 112:535–542, 1977.

[2] Kuhara, S., Satou, K., Furuichi, E., Takagi, T., Takehara, H. and Sakaki, Y., *"A deductive database system PACADE for the three dimensional structure of protein"*, Proc. of the 24th HICSS, 1:653–659, 1991.

[3] Satou, K., Furuichi, E., Takiguchi, K., Kuhara, S. and Takagi, T., *"Application of a Deductive Database System PACADE toward Discovery of Clusters of Similar Structures in Proteins"*, Proc. of the 27th HICSS, 5:160–169, 1994.