Enhancement of the "PROTEIX" Database System for Three-Dimensional Protein Structures

Tatsuya Akutsu [1] Toshio Hyakutake [2]

akutsu@cs.gunma-u.ac.jp

[1] Department of Computer Science, Gunma University
1-5-1 Tenjin, Kiryu, Gunma 376 Japan

[2] Fukuoka Industrial Technology Center
3-6-1 Norimatsu, Yahatanisi-ku, Kitakyushu-shi 807 Japan

Abstract

We have been developing a protein structure database system named PROTEIX. In this report, we describe recent improvements on PROTEIX.

1 Introduction

In the last year, we have reported the development of a database management system for 3D protein structures, named PROTEIX (PROTEIn database system on uniX) [1]. PROTEIX has become more useful since several improvements have been done in this year.

2 Improvements

One of the features of PROTEIX is that it has a function (*substructure search*) for searching for similar fragments of protein structures. The previous substructure search algorithm was replaced by a new algorithm [2]. It is several times faster than the previous one. Moreover, new data structure, which enabled all protein structure data to be stored in main memory, was implemented. Due to these improvements, a substructure search among 811 protein structures can be completed within a few seconds on a SUN SPARC Station-10.

The user interface has been considerably improved by adopting the OSF/Motif system. Moreover, a file selection box is newly appended, which appears on the right of the display window (see Fig. 1). Users can specify a PDB file using it, and PDB files found by a substructure search are displayed on it.

[1]阿久津達也：群馬大学工学部情報工学科，〒376 桐生市天神町 1-5-1
[2]百武稔郎：福岡県工業技術センター，〒807 北九州市八幡西区則松 3-6-1

Acknowledgement

This work was partially supported by a Grant-in-Aid for Scientific Research on Priority Areas "Genome Informatics" of the Ministry of Education, Science and Culture in Japan.

References

[1] T. Akutsu, "PROTEIX: an interactive database system for three dimensional protein structures," *Proc. Genome Informatics Workshop IV*, pp. 430-433, 1993.

[2] T. Akutsu, K. Onizuka and M. Ishikawa, "New hashing techniques for three-dimensional protein structures," to appear in *Proc. Genome Informatics Workshop V*, 1994.

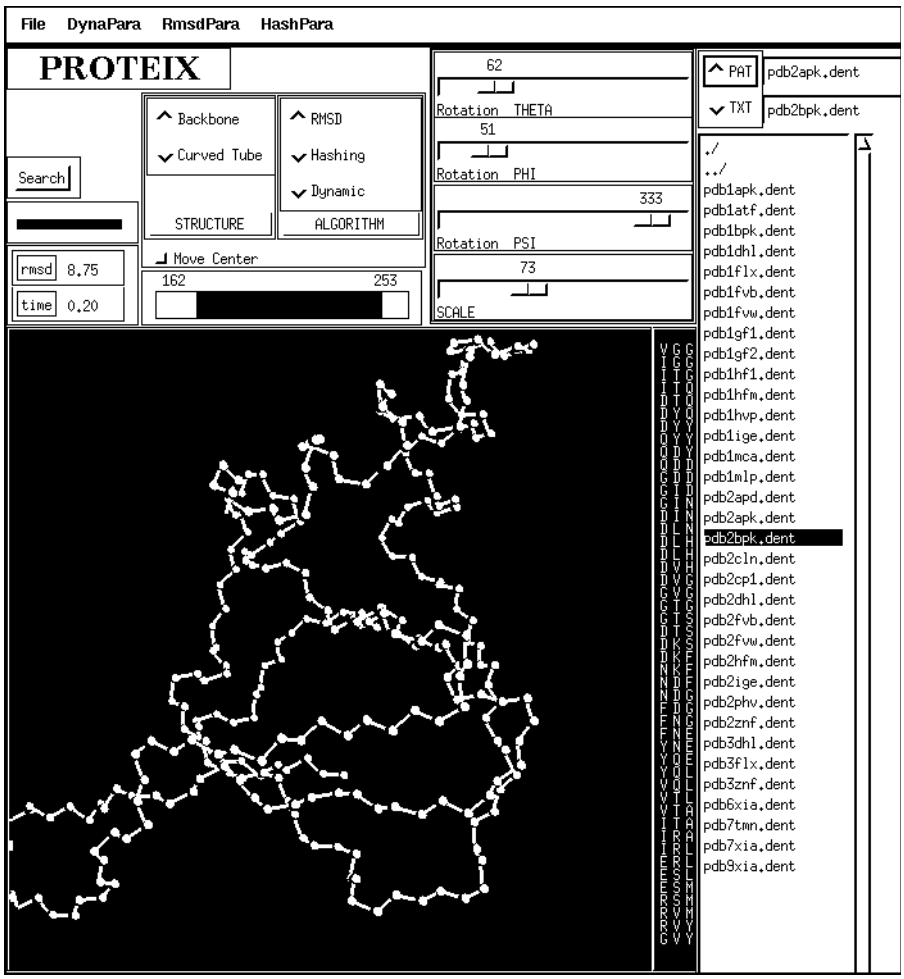

Figure 1: Snapshot of PROTEIX. Note that pictures appear on a color display in the real system.