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Protein Disulfide Bond Database

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Abstract

In the first year of our two-year project, we have built a database of disulfide bond classification of protein.   At the present stage, our system offers keyword search of disulfide bond patterns, PDB code, disulfide numbers and cystein motif.Our database is derived from PDB database, DSSP, HSSP and FSSP. The preliminary SSDB is available at http://because-c.life.nctu.edu.tw/~ssbond .

Introduction

Disulfide bonds are important both in structure and function of many proteins, they can stabilize the folded state either enthalpically through favorable local interactions, e.g., by stabilizing the packing of a local cluster of hydrophobic residues, or entropically by reducing conformational space of the unfolded form. Experimentally, disulfide species are usually rather stable, so they can be relatively easy to be isolated and characterized structurally. Hence, it is rather surprising that there is not yet a specialized database for the classification of disulfide patterns of protein. Here we present a database of disulfide bond classification of protein, which will be referred to as SSDB.

Methods

SSDB is based on Protein Data Base and other databases related to classification 2nd structure such as DSSP, HSSP and FSSP. Most of the software was built using the PHP scripting language. We also use the MySQL relational database management system, which is known to be fast, reliable, capable of handling large data sets, and

free for non-commercial. Our system will automatically update the relevant databases such as PDB, HSSP, etc, weekly. Our software is highly portable, and should be able to run on any Linix/BSD/UNIX systems.

Results and Discussions

The current statistics of disulfide proteins is shown in Fig. 1. The number of disulfide bond number decreases drastically at 5 or more. The largest disulfide bond number of proteins deposited in PDB is 17. The SSDB web page is show in Fig. 1. At the present stage, users can make queries about the number, pattern of disulfide bonds, SS-containing proteins in PDB. One of the search results is shown in Fig. 3, when the user query about the proteins containing 15 disulfide bonds. The web page shows the number of patterns and PDB codes. We also offer Chime user interface in our page so that users can display 3D graphics of the proteins and visualize the disulfide bond patterns(see Fig. 4). In the first, we have successfully build disulfide bond classification protein database. In the next year, we will develop predictive tools and extend our databases to include SWISSPROT and PIR.

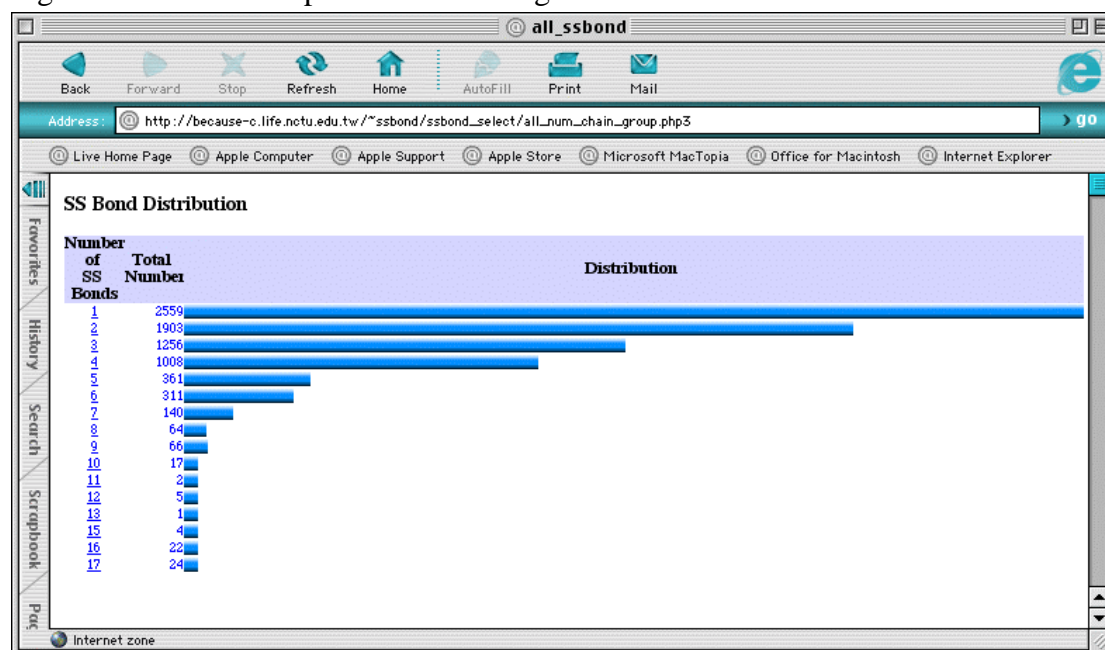Fig. 1 The statistics of proteins containing disulfide bonds in PDB
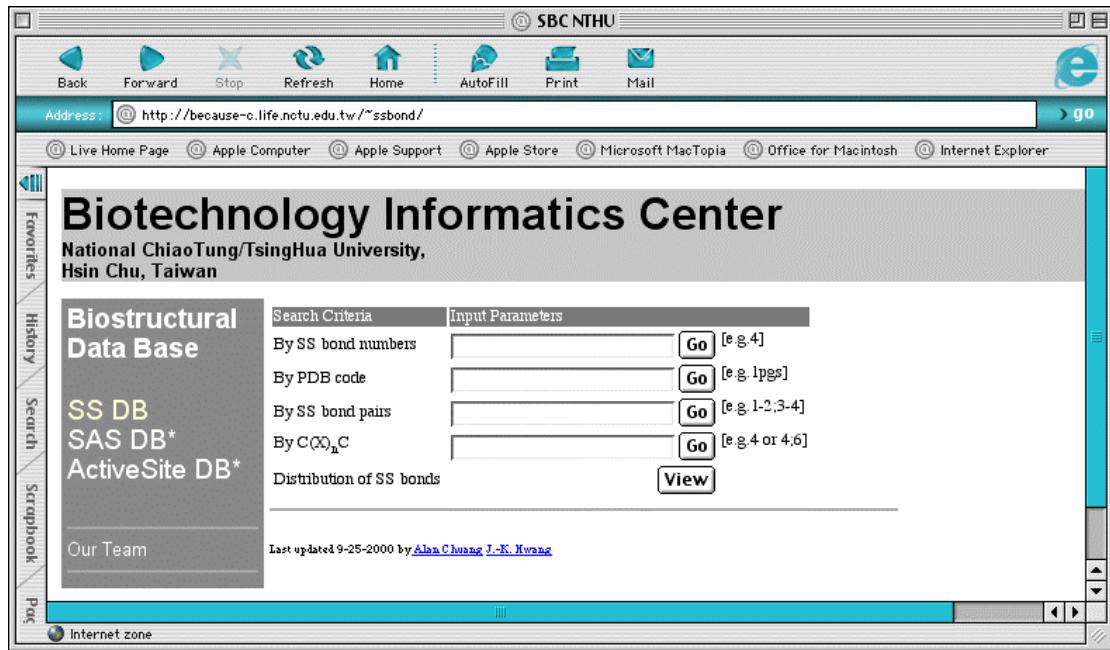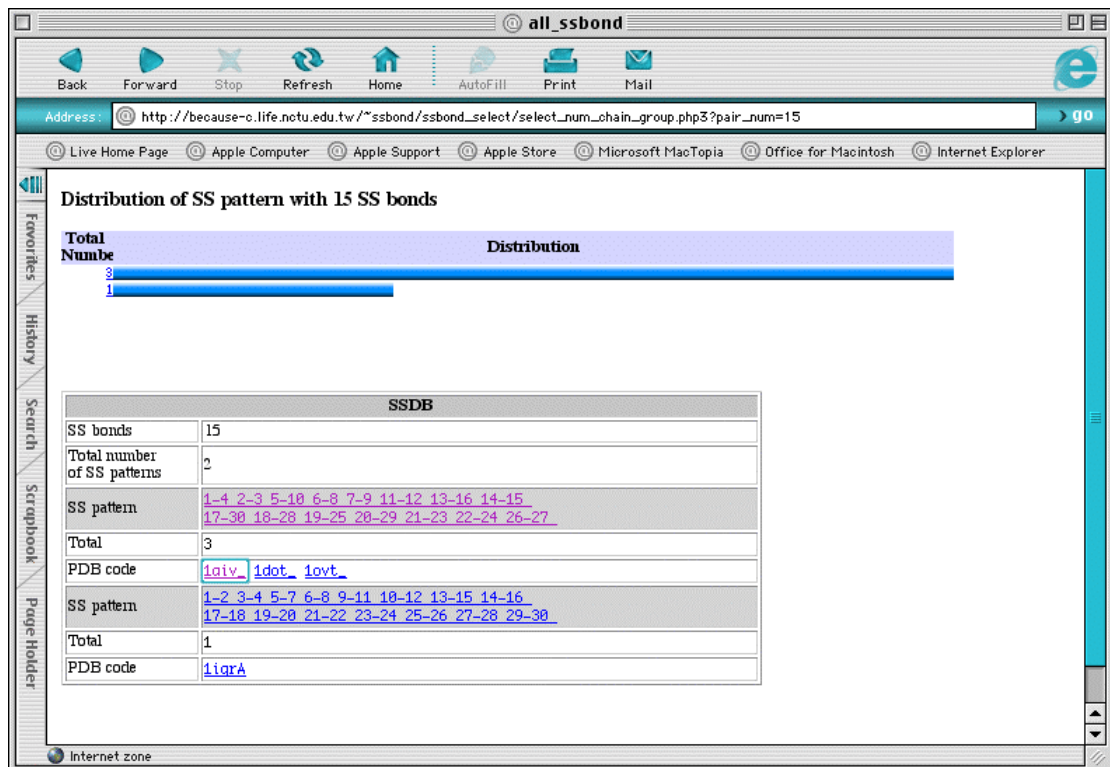
Fig. 2. The webpage of SSDB

Fig. 3 The query results returned by SSDB

Fig. 4 Chime user interface in SSDB