

Poster I-88

Protein Structural Analysis Made Easy



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Short Abstract: Biologists do not always have the appropriate training to do in silico analysis of protein structures. We aim to provide a one-stop, browser-based tool and visualization facility, which will allow the user to analyse protein structures and retrieve data about the protein via webservices from other international sites.

Long Abstract:

Biologists do not always have the appropriate training to do in silico analysis of protein structures. We aim to provide a browser-based tool to assist biologists in carrying out extensive in silico analysis of protein structures. The primary function of this tool is to allow the user to store and manage their data and results in one centralized place. It will provide browser-based visualization capabilities via Jmol as well as RPC-linked access to a local installation of PyMol. Information from databases (up-to-date local mirrors) such as Uniprot, PDB and Pfam will also be available and will be displayed on the protein via plugins written for PyMol. A user will also be able to run secondary structure predictions on any submitted or stored sequence. The user will also be able to store models and protein structure files. Information regarding all levels of protein will be provided from databases such as CATH and SCOP. It will also provide script generation tools for CHARMM and Modeller as well as guided, step-based methods for analysing the effect of mutations of structures. This will allow the user to start analysing and modelling proteins much quicker as it cuts out the need to learn the syntax of new programs.

This tool will form part of the FunGIMS project currently in development at the University of Pretoria and will be written in Java within a Struts framework, running on Tomcat with a MySQL backend. To store the protein data, it was decided to use the Uniprot-XML schema and protein structural data, PDBML.

In a low bandwidth and technology poor country such as South Africa, this centralized way of analysing and storing data provides an efficient way for biologists to manage and analyse their data. It also overcomes the limitation of needing higher end desktop machines to do analysis (which is mostly not affordable in South Africa).