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Structural Annotation Pipeline for Malarial proteomes

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Short Abstract: The pipeline consists of a series of established bioinformatics tools, such as Blast vs. PDB, family assignment, secondary structure and TM predictions, and is applied to several malarial proteomes. Annotations such as protein interactions and small molecule interactions are added for P.falciparum. Results are made accessible through a web application developed in ZOPE.

Long Abstract:
Protein Structural Annotation Pipeline for Malarial proteomes

In silico structural studies are becoming increasingly important and a large range of different bioinformatics tools are available for these structural studies. P.falciparum is the species responsible for the most lethal form of Malaria. With the completion of the P.falciparum genome project, much data is available for mining. This project focuses on combining various established bioinformatics tools for structural annotation of Malaria proteins in a comprehensive searchable database. The pipeline performs a series of high-throughput analyses, using Python-MPI as a wrapper to analysis of ORF's using existing applications on a 64-node Linux cluster. Analyses include screening against PRINTS and Prosite, several EMBOSS modules, Blast search vs PDB, HMMER searches against Pfam, Superfamily and BLOCKS databases. Various secondary structure prediction methods and transmembrane-helix analysis using TMHMM are included. Three dimensional structure prediction using Threader will also be added to the pipline. The results are stored in a PostgreSQL database. The results will be made publicly available in the form of a web-accessible frontend to the database. The web application is developed using the ZOPE platform.

To select proteins suitable for structural studies such as homology modeling and docking studies, other annotations such as protein-protein interactions, small molecules predicted to bind to proteins, proteins predicted to be exported to the RBC according to presence of a PEXEL motif, proteins containing inserts, having an existing three dimensional crystal structure or homology model are also included for P.falciparum proteins. P.falciparum proteins can then be selected via the web interface according to the presence or absence of one or more properties. Known inhibitor annotations are to be added to the database.

For structural feature comparison to other species, other Malarial species (P.vivax, P.yoelii and P.chabaudi) as well as H.sapiens proteins have also been annotated by the structural annotation pipeline and results for the protein homologues of P.falciparum can also be viewed.

The database will aid in selecting suitable targets for structural studies of Malaria proteins like homology modeling, crystallization studies and docking studies. Targets can be identified based on a range of conditions the user selects himself. The structural annotation pipeline can easily be extended to other genomes.