Abstract

English

The crystallisation of proteins for X-Ray diffraction can be a long lasting and exhausting task. Usually many parameters like the pH, the temperature and the concentration of the additives are varied to grow a crystal. The here developed application allows to calculate, store, view and analyse surface attributes and protein-protein crystal contacts for proteins with a known structure and should lead to a better understanding of protein contacts and their crystallographic and biological function. This understanding can later be used for the design of protein mutants with better crystallisation premises or the search for biological protein-protein interaction partners.

The three tiered Java enterprise application was developed using model driven architecture. The database schema is based on the Protein Data Bank. It has been enhanced by tables to store protein surfaces, contact patches and various properties including hydrophobicity and electrostatic potential of surface points and contact regions. Detailed interfaces and an underlaying task management have been designed for import functions, calculations and analyses. All business methods can be accessed through a Web interface based on the Model-View-Controller framework Struts. Oracle was used as database server and JBoss as application server.

Keywords: protein protein interaction, crystal contacts, database, J2EE