Protein Structure Database and Visualisation System

Proasis3: Making the most of your Protein Structure Data

Links data, methods & scientists

Designed for MedChem

Customizable

Fast

Powerful

Robust

Easy to use

Collaborative

Effective visualization

Sophisticated modelling methods

DATA SUBMISSION

Streamlined

Automated

Straightforward

COMPLEX DATA HANDLING

Explicit Visualisation

Allows in-house & PDB data

Data Curation

Structure validation

Access to expert methods via easy to use interface

MODELLING METHODS

ViewContacts Interactions

Scorpion Scoring

Viper Ligand Design

CQDB Non Covalent Interaction Searching

Felix: Binding Site Similarity Searching

ProFusion Session Files

Receptor Flexibility Analysis

Kinase Data Mart

WaterView: Water Clustering

Proasis3 is a robust, automated database with an easy-to-use interface ,
powerful research* methods *and visualization tools

Typical Protein Structure Data Problems:

Highly complex requiring significant expertise

Large quantities of varied, often poor quality data

Constantly updated and modified

Difficult and time consuming to submit

Disparate Information resources

File format limitations

Reliable chemical information hard to access

Oligomeric systems require special attention

Ligand binding modes challenging to understand

Proasis3 addresses all of these issues in one easy to use system

Structure Deposition made easy:

Precise and accurate structure submission is critical for drug discovery applications. It is often overlooked due to it's time consuming and tedious nature. Proasis3 solves this issue. Multiple methods are available for loading structures into the Proasis3 database including webGUI, command line scripts and fully automated methods.

Web based structure deposition minimises the burden on (

fields . Key data is obtained from the pdb file and previously submitted structures. Fully automated methods can also be used to load the database for both in-house and public domain structures, in turn, transforming the submission process.

DesertScientific
Software
www.desertsci.com

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Proasis3 Manages Hard Structures

Specifically designed deposition tools effectively handle harder in-house protein crystal structure data.

Binding site regions in both liganded and un-liganded structures can be located

All mononmers in homo-multimers automatically identified

All proteins in hetero-multimers automatically identified

Binding sites with multiple ligands carefully handled

Protein chains with multiple binding sites carefully handled

OTHER FEATURES

Stores in-house , public domain, X-Ray , NMR and modeled structures in RDMS (either Oracle or MySQL)

Wide range of browsers and graphics packages supported

Projects viewed as a hierarchical tree giving a MedChem view of data

Able to store

- Sstructure factor files
- Topology files
- Parameter files
- Scaling log files
- Map files
- Supplementary data files
- Reports
- Presentations
- Images
- … and much more

Creates deposition reports for ELN systems

Storage and visualization of electron density maps

On-the-fly creation of electron density maps from structure factor files

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ZERO DOWNTIME

Ut wisi enim ad minim veniam, quis nostrud exerci tation

Binding sites at the interface of multiple chains can be managed

Profusion Session Files

ProFusion is our technology for generating comprehensive session files for any project. The modeller sets up the initial the ProFusion session file, based on their project expertise. Thereafter, it is automatically maintained.

All small molecules ass cor

Support

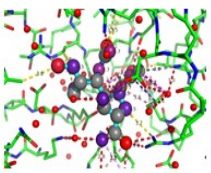
Adminis

Why Proasis3?

Proais3 is a complete system that combines a superior relational database for storing, retrieving and searching structures important to MedChem projects, with the most intuitive desktop visualisation system for exploring those structures. Proasis3 provides significant flow-on effects improving internal productivity, efficiency and communication through your research organisation. Proasis3 provides linkages to DesertSci's proprietary modelling methods ViewContacts, Scorpion, Viper and ProFusion. Proasis 3 is designed, in collaboration with pharma R&D researchers, to extend the range of possibilities for scientists to think, design and create.

Proasis3 is Fast, Powerful, Easy

… like surfing the web



System Requirements

- Server software runs on Linux
- Client software runs on Windows, Mac, Linux
- RDMS: Oracle or MySQL
- Industry standard desktop PC
- Supports most major graphics packages
- Supports all major browsers

DesertScientific Software
www.desertsci.com