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**

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

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

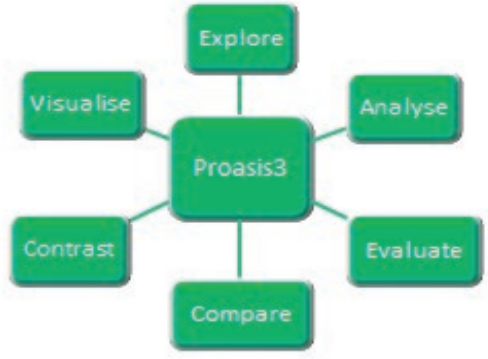
MODELLING METHODS

- 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

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 crystallographers . Submission involves filling just a few 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

⇒ Binding sites at the interface of multiple chains can be managed

⇒ All small molecules associated with a protein structure file are comprehensively managed and ligands in binding sites differentiated from other small molecules

⇒ Supports all older and newer pdb file formats

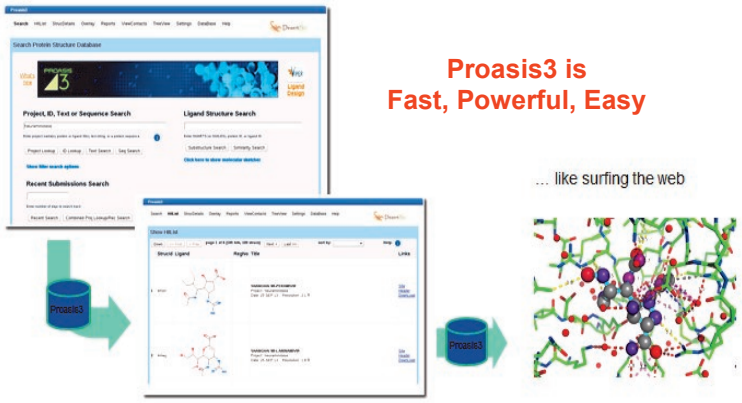
⇒ Administration tools for easy updates

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.

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.



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

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