

# Proasis3™

## A Fast, Responsive Informatics System for Drug Discovery

Proasis3 is a new Rich Internet Application (RIA) built on top of the Proasis2 database and visualization system. It integrates data and methods with design and technology to help you achieve your informatics goals.

Proasis3 is a:

- **Rich Experience** – we have set the focus to *'how can we better help users get more'*
- **Rich Functionality** – it acts like a **desktop** application but has all the benefits of a browser application
- **Rich Client** – **leverages** the growing power of client machines and modern browsers
- **Rich Communications** - allows data to be retrieved from the server without page reload making it **faster and more user-friendly**

Finely tuned to work in concert with the Proasis2 database, Proasis3 is packed with powerful new features to improve flexibility and user experience. In one complete system it combines a superior relational database for storing, retrieving, and searching structures important to medicinal chemistry projects with the most intuitive desktop visualization system for exploring those structures. Proasis3 provides significant flow-effects improving internal productivity, efficiency and communication throughout your pharmaceutical research organization.

Developed using open source **state-of-the-art** technology such as Google Web Toolkit, Pyjamas and PureMVC python, Proasis3 responds instantly for users and improves real time productivity. Built to be **'future proof.'**

Proasis3 provides linkage to DesertSci's proprietary **ViewContacts** software giving you access to superior tools for exploring protein-ligand interactions.

Proasis3 provides linkage to DesertSci's proprietary **Scorpion** software giving you access to our ground breaking scoring function and ligand binding analysis tools.

Proasis3 is designed to expand the range of possibilities available for scientists to think, design and create whilst remaining a flexible and easy-to-use system. It is **technology at work for you.**

### Proasis3 – KEY FEATURES

- Highly customizable
- Browser application that works like a desktop application
- Minimizes client server communications
- Intuitive, web-based user interfaces
- Portal to ViewContacts and Scorpion software
- Easy to use and easy to maintain
- Includes fine tuned checking of input parameters
- Use of Speed Tracer for Chrome to achieve maximum performance
- Runs highly optimized javascript – is fast and easy to load in all popular browsers on the main platforms.
- Flexible, scalable, robust
- Comprehensive on-line help
- Fast to implement new features
- GWT/pyjamas means **just one version of code** is needed to support multiple browsers
- Comprehensive test suite base on selenium

## Proasis3: A Rich User Experience

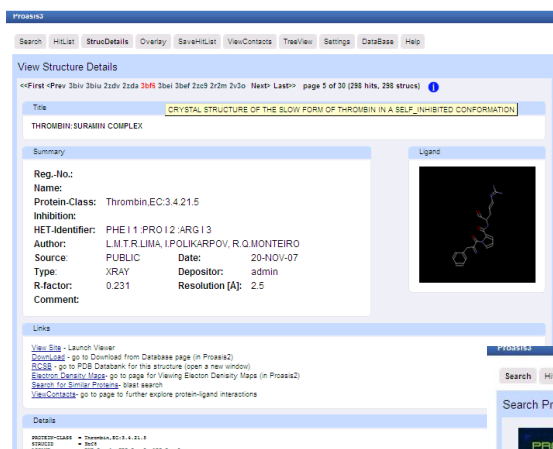
### Works like a Desktop Application

Proasis3 is a browser application that works like a desktop application.

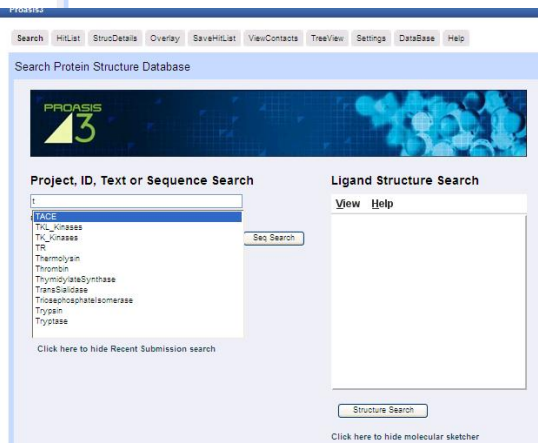
- Hitlists can be re-sorted according to different properties and re-sized **dynamically**, entirely on the client.
- The desktop application retrieves data from the database more **efficiently** using asynchronous javascript technology. This means data can be retrieved in the background without interfering with the display and /or behaviour of the existing web page.
- More data can be stored on the client, making navigation **faster**.
- Tooltips and PopUps link directly to helpful hints
- Hitlists can be pruned or extended; rows easily **customized**, selected and manipulated.
- more data can be more **easily** explored and used

### Improved Look and Feel

Proasis3 provides structure information with all the familiar details and functionality of Proasis2 but with a new and improved look. There is faster browsing from one structure to the next enabling a **richer user experience** and greater productivity. Proasis3 continues to provide a medicinal chemistry view of protein structure data enabling structures to be classified so that chemists can easily browse all protein-ligand complexes associated with their project(s). The new interface is **intuitive, fast** and **simple to use** making complex tasks routine.



*Proasis3's new look  
and improved  
searching  
functionality provides  
fast and accurate data  
retrieval*





## Text Searching Made Easy

Proasis3 **connects you to the information you need** by making text searching even easier.

- With inbuilt auto-completion simply type the first letter and all projects starting with that letter are listed. Just select one and click Project Lookup and all project structures are retrieved - **simple, fast, effective**.
- There is new, fast searching using compound ID numbers or just the last few digits of a compound ID or set of IDs.
- All searches are accessed from just one page of the interface and users have the option of selecting their preferred molecular drawing package.

## More Options Equals More Productivity

Powerful new options are available with Proasis3:

- Users can choose their preferred molecular drawing package
- Hitlists can be extended and/or pruned
- End-user settings can be saved from one session to the next
- The project tree is fast to load and navigate and the state is maintained
- Project summaries can be quickly retrieved and inspected
- Structures from any project, or set of projects can be retrieved at the click of a button.

**Proasis3 allows you to unlock the value in your data**

*More options for hitlists,  
end user settings, project  
summaries – Proasis3 is  
productivity in motion*

The image displays three screenshots of the Proasis3 web application interface. The top screenshot shows the 'Show HitList' page with a table of search results. The table has columns for 'StrucId', 'Ligand', 'RegNo', and 'Title'. Three entries are visible: 41 3biv, 42 3biu, and 43 2zdv. Each entry has a corresponding molecular structure image. The middle screenshot shows the 'Settings' page, which allows users to configure various options such as 'New Hits', 'Chemical Drawing', 'Select Viewer', 'Search Space', 'Protein-Class', 'Structure Type', 'Structure Source', 'Display Style', and 'Hits per page'. The bottom screenshot shows the 'Tree View of Project Hierarchy' for a selected project named 'PPAR\_A'. It displays a tree structure of sub-projects and a 'Project Summary' box with statistics like 'Structure Source - total, inhouse, public: 12, 0, 12' and 'Number of complexes/unliganded: 12, 0'.



## Proasis3: Rich Functionality

### Portal to ViewContacts™

ViewContacts is proprietary, **state-of-art software** giving chemists, modelers and crystallographers a superior understanding of non-covalent interactions in protein-ligand complexes. All non-covalent interactions in a protein-ligand complex can be thoroughly explored using the links between Proasis3 and ViewContacts. An additional client application provides identical functionality for non-database structures, such as docking results and structures generated from interactive modeling sessions.

Additional functionality for interactions include:

- Easy viewing of fine grained representations of non-covalent interactions
- Highlighting of all contacts in a binding site
- Display of contacts involving only those residues in very close proximity to the ligand
- VCWeb a desktop application for non-database structures such as docking results and structures generated from interactive modelling sessions is also available.

For more information on ViewContacts please refer to our brochure.

### New Viewing Features

Proasis3 has been extended to allow enhanced PyMol viewing all in one session

- The binding site view includes the entire contents of a pdb file
- Alternative conformations are highlighted in the binding site
- All symmetry molecules making contact with the binding site are shown
- Fine-tuned protein-ligand interactions are illustrated, including unfavourable contacts

**Proasis3 is smart technology at work for you.**

### Enhanced Overlay Functionality

- Larger numbers of structures can now be superimposed in one session
- Overlaid structures can be exported as a set of pdb files
- Protein-ligand interactions can be viewed for overlaid structure
- Size of binding site easily fine tuned
- You can now make use of PyMol's inbuilt optimized alignment algorithms.

*Proasis3 has the  
functionality to help  
keep you at the  
cutting edge*

The screenshot displays the Proasis3 web interface. On the left, a panel titled 'Further Explore Non-Bonded Interactions' allows users to filter and group interactions. It includes options for 'Display Interactions' (protein-ligand or all in binding site), 'Grouping of Interactions' (a dropdown menu), 'Buried Interactions' (show buried and unburied or only show buried), and 'Size of Binding Site' (a dropdown menu). A 'Run ViewContacts' button is present, with a note 'Calculation may take up to a minute'. Below this is a 'Ligand' section with a 3D ball-and-stick model of a ligand (labeled 'Sdux'). The main central area shows a 3D molecular model of a protein-ligand complex with various interactions highlighted. On the right, a 'Structure Overlays' panel provides a four-step process: 1. Select Structures, 2. Select Reference, 3. Select Overlay Method (with a link to 'PyMol optimized sequence alignment'), and 4. Prepare Structures. A 'Setup Overlay' button and a link to 'Click here to launch PyMol' are also visible.



## Customization

Proasis3 is developed using the Python programming language. It is extremely powerful, simple, elegant, clear, safe, and fast. The latest technology has been used including:

- GWT – Google Web Toolkit the most powerful toolkit for creating Ajax applications
- Pyjamas – the Python version of the GWT
- PureMVC Python – a powerful framework based on Model View Control software architecture

This combines to make Proasis3 easy to customize to your specific needs and design requirements. It also ensures the system remains easy to maintain, extend and upgrade either in-house or through an ongoing maintenance agreement with DesertSci.

## Hardware and Software Requirements

Industry standards:

- Proasis2™ server software is required, runs on Linux
- clients can use MS Windows, Apple Mac, and Linux
- typically, Proasis3™ will work on an industry standard desktop PC without any specific configuration requirements
- protein structures are stored and retrieved as pdb files; indexed and annotated in Oracle or MySQL
- front-end 100% JavaScript
- all major browsers supported
- major graphics packages are supported, including PyMol, Chime, DS ViewerPro, RasMol, MOE, and Benchware 3D Explorer

Contact Us: [info@desertsci.com](mailto:info@desertsci.com)

[www.desertsci.com](http://www.desertsci.com)

Evaluation Licenses Available