Proasis 4

Design Platform

Proasis4: A Design Platform for 21st drug discovery

DATA SUBMISSION

- Streamlined
- Automated
- Straightforward

COMPLEX DATA HANDLING

- Explicit Visualisation
- Allows in-house & PDB data
- Data Curation
- Structure validation
- Access to expert methods via adaptable interface

MODELLING METHODS

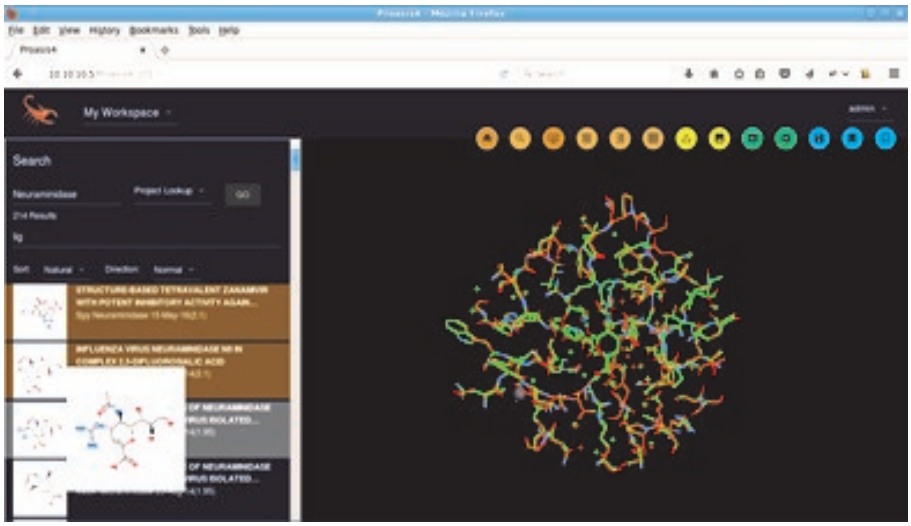
- API Client Tools
- ViewContacts Interactions
- Scorpion Scoring
- Viper Ligand Design
- CQDB Non Covalent Interaction Searching
- Felix: Binding Site Similarity Searching
- Extended ProFusion Session File capability
- Receptor Flexibility Analysis
- Kinase Data Mart
- WaterView: Water Clustering

TURNKEY SOLUTION

- Can be easily implemented into any research infrastructure
- Designed to be used immediately to enhance drug design and discovery

- **Built on the powerful ProasisAPI**
- **UX designed user interface**
- **Built-in 3D molecular graphics**
- **Expansive database with increased data hierarchy**
- **Extended searching capability**
- **Sophisticated design methods**
- **Build/share/extend sessions**
- **Precise, Robust, Scalable, Fast**

Proasis4 is a powerful design platform that couples an expansive database with a beautifully designed interface to meet the modern demands of drug discovery



Proasis4 has been transformed into a design platform from a database and visualisation system. We have deliberately moved from a search/retrieve/handle system to a design philosophy based on interactivity. Proasis4 is built on our powerful ProasisAPI. This allows users to access advanced functionality and features both, within Proasis4, and across other company licensed software. The result is better integration of **all** your methods and tools across the research environment.

DesertScientific
Software
www.desertsci.com

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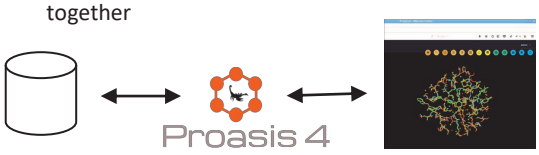
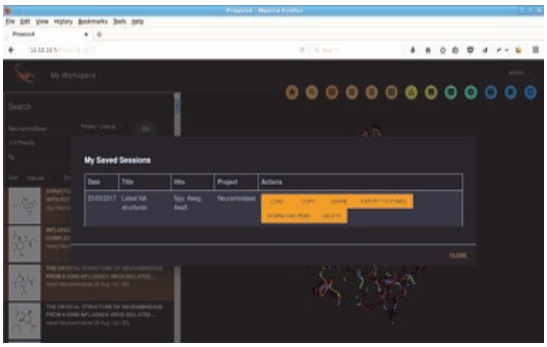
Why Proasis4?

- Proasis4 is a drug **design** platform. It provides a group of technologies upon which you can design better and more innovative drugs.
- Proasis4 is about **interactivity** with the database, and bioinformatics tools and methods. We have significantly increased the hierarchy of data. This means each experimental structure is even more closely defined, allowing for greater agility and innovation in how you put your drug design ideas together

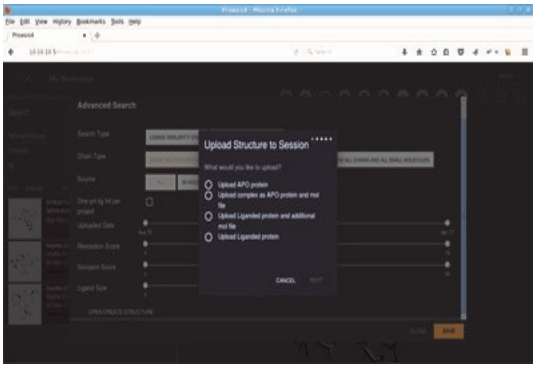


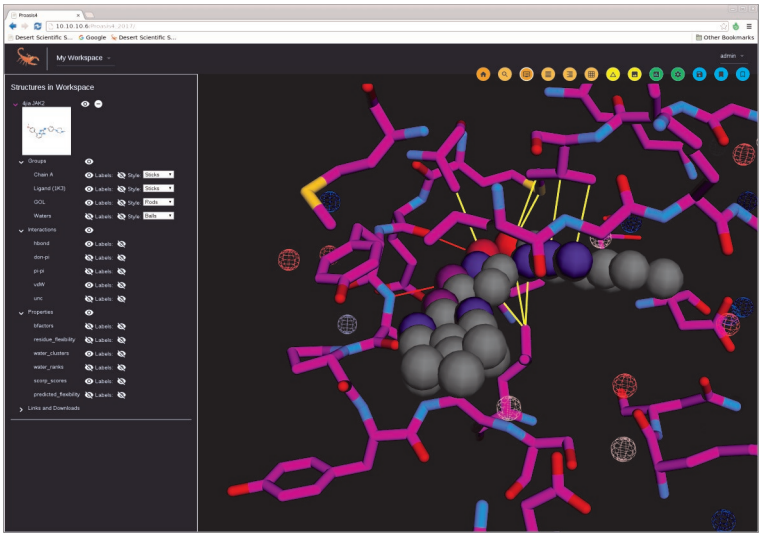
- Proasis4 champions **innovation**. It lets you read non-database structures into the platform. You can design a ligand, add it to the platform, access Proasis4 methods and then compare and contrast to existing database experimental structures dynamically. By creating this design process of experimentation and prototyping, Proasis4 enables you to embrace innovative design as a core competency.
- Proasis4 focuses on **flexibility**. It allows for dual connectivity between the database and the Proasis4 search engine and visualisation. This means you can work seamlessly across technologies in real time, without the need to launch and re-launch software.



Proasis4: Build/Share/Extend sessions

Proasis4: Extended searching capability





Proasis4: Built for MedChem projects

OTHER MAIN FEATURES

- Stores in-house, public domain, X-Ray, NMR and modelled structures in RDMS (Oracle or MySQL)
- Knowledge based analysis and property prediction
- Projects in hierarchical tree giving a MedChem view of data
- Extended support for Biologics
- Extended generation of macro - molecular assemblies
- Enhanced field searches eg. regular expression
- Able to read in local structures for comparison
- Able to use modelling methods and tools on local structures
- Able to store
  - Structure factor files
  - Topology files
  - Parameter files
  - Scaling log files
  - Map files
  - Supplementary data files
  - Reports,Presentations,Images
- Creates deposition reports for ELN systems
- Storage and visualisation 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
- Supports all major browsers

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