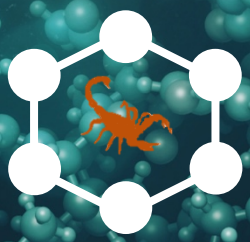


Proasis4

FIRSTLY

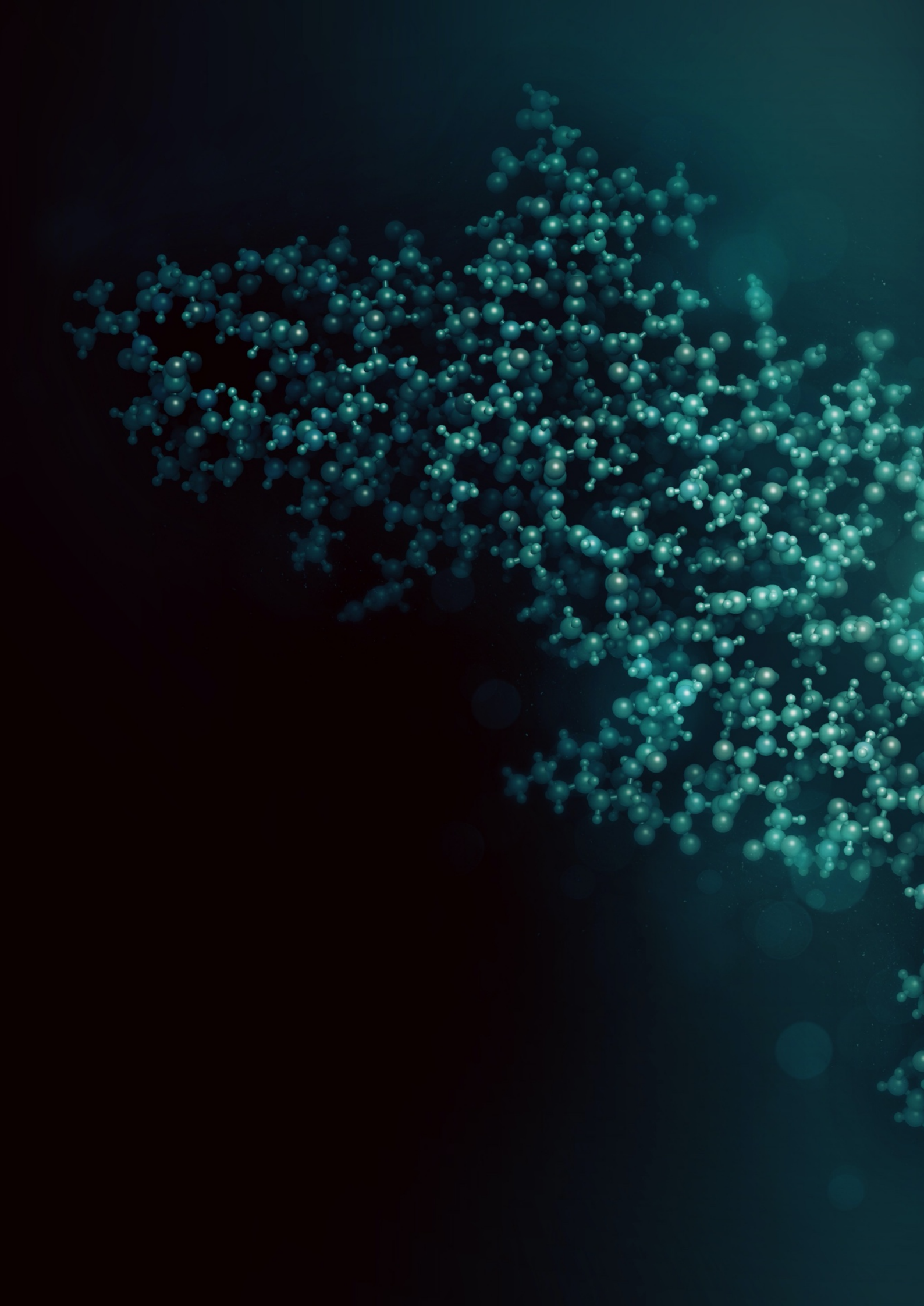
WHAT IS PROASIS?

Proasis is a powerful drug design platform. It couples an expansive database with an intelligently designed graphical user interface. The combination of these features culminate to meet the contemporary demands of drug discovery.

Proasis4 has been redesigned around our powerful Proasis API. This allows users to access advanced functionality and features within both Proasis4 *and* third-party licensed software.

The result...Better integration of all your methods and tools across your research environment.

CONTENTS



1 | INCLUSIONS

DATA SUBMISSION

- → inhouse & PDB data
- → xray, NMR, modelling & CryoEM structure
- → streamlined
- → automated
- → straightforward

COMPLEX DATA HANDLING

- → explicit visualisation
- → data curation
- → structure validation
- → multiple overlay methods
- → access to expert methods via adaptable interface

TURNKEY SOLUTION

- → can be easily implemented into any research infrastructure
- → designed to be used immediately to enhance drug discovery

MODELLING METHODS

- → API client tools
- → ViewContacts interactions
- → Scorpion scoring
- → Viper ligand design
- → FELIX non-covalent interaction searching
- → FELIX: binding site similarity searching
- → ProFusion session file capability
- → Receptor flexibility analysis
- → Kinase Data Mart
- → Waterview: water clustering

PROASIS FEATURES

knowledge based analysis and property prediction

stores in-house & public domain: xray, NMR, CyroEM and modelled structures in RDMS (Oracle or MySQL)

projects in hierarchical tree giving a MedChem view of data

advanced search capability including: project, compound ID, chemical structure, sequence, text/keyword, date

able to store and share:

- → protein structure files
- → chemical structure files
- → structure annotation
- → topology files
- → parameter files
- → scaling log files
- → map files
- → fasta files
- → spreadsheets
- → supplementary data files
- → reports
- → presentations
- → images
- → mmcif and cif files
- → session files
- → ligand design results

able to use modelling methods and tools on local structures

able to read in local structures for comparison

visualisation of atom based ligand affinity scores

create deposition reports for ELN

extended handling of Biologics including antibody classifiction & clustering; CDR annotation

storage & visualisation of electron density maps

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

extended generation of macro-molecular assemblies

WHY PROASIS?

DESIGN

Proasis is a drug **design** platform. It provides a group of technologies on which you can design better and more innovative drugs.

INTERACTIVITY

Proasis is about **interactivity** with the database, cheminformatics/ bioinformatics tools and methods. A fine-grained project hierarchy allows for greater agility and innovation in how you put your drug design ideas together.

INNOVATION

Proasis champions **innovation.** It lets you read non-database structures into the platform. You can design a ligand, add it to the platform, access Proasis methods and compare/contrast to existing database experimental structures dynamically. By providing this design process of experimentation and prototyping, Proasis enables you to embrace innovative design as a core competency.

FLEXIBILITY

Proasis focuses on **flexibility**. It allows for dual connectivity between the database and the Proasis search engine and visualisation. This means you can work seamlessly across technologies in real time, without the need to launch and re-launch software.

SYSTEM REQUIREMENTS

SYSTEM REQUIREMENTS

- Server software runs on linux
- Client software runs on Windows, Mac, Linux
  - workstations
  - laptops
  - tablets
  - smartphones
- RDMS: Oracle or MySQL
- Supports all major browsers

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