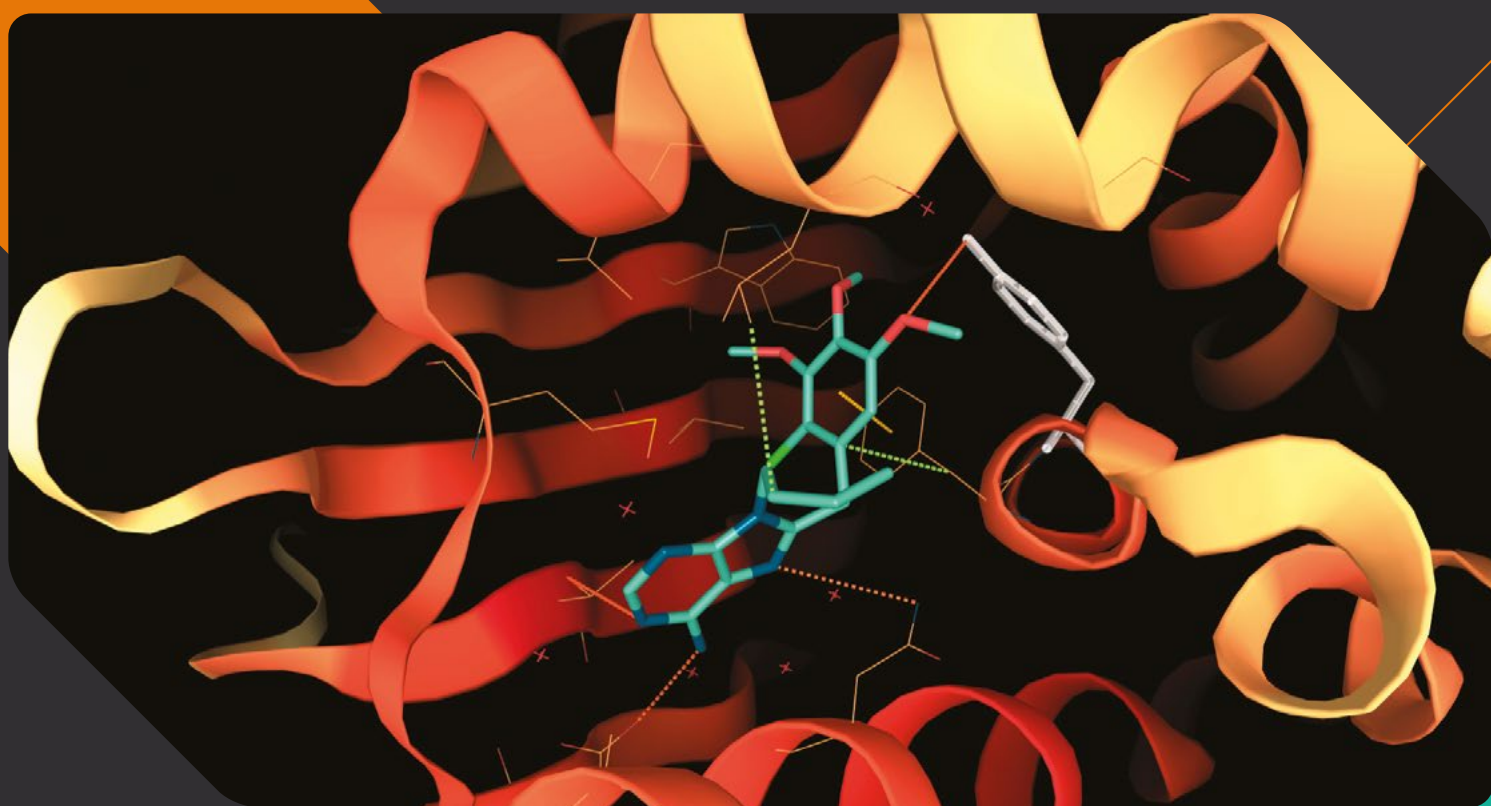


Release
the full potential
of your 3D
biomolecular
structures



3ddecision



A Collaborative Platform for Structural Knowledge Management



UNIQUE INSIGHTS
INTO PUBLIC AND PRIVATE
BIOMOLECULAR
STRUCTURES

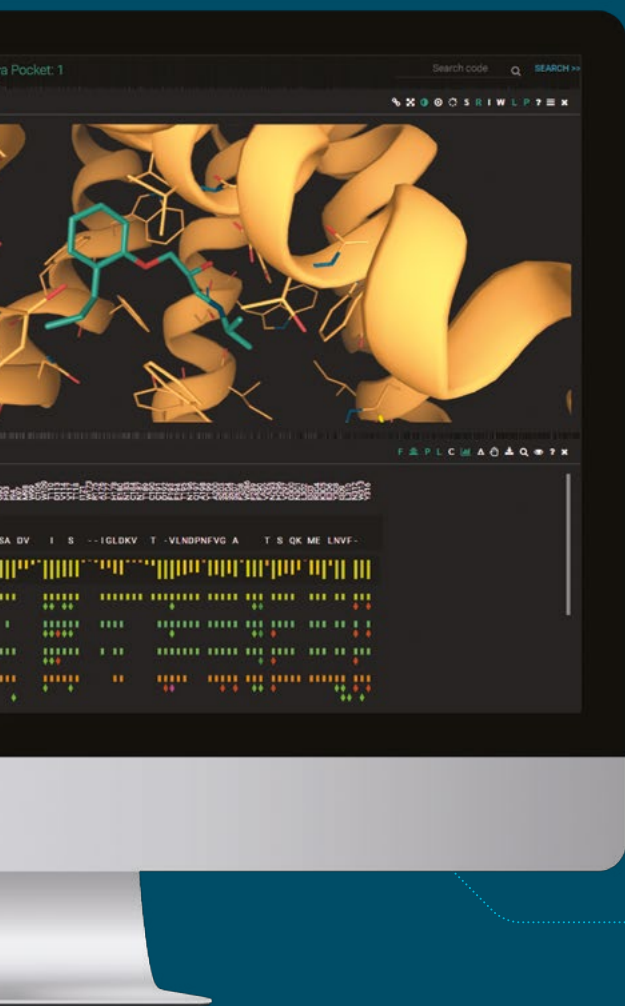


INTERDISCIPLINARY
COLLABORATIVE
ENVIRONMENT



MODERN WEB
APPLICATION
WITH DISRUPTIVE UI

discngine



Capitalize more on structural data!

3decision addresses four major pitfalls in today's structure-based drug discovery projects.

Capture and sustain structural knowledge seamlessly

In 3decision, public & proprietary structures, experimental structures & derived models are all automatically analyzed, organized and imported into a unique database.

Tap into large-scale structural analysis

In 3decision, large-scale structural analysis is easily accessible thanks to a unique data model and advanced algorithms.

Push advanced structural searches further

In 3decision, use text, molecular fragments, pocket similarity, interaction patterns or any other structural entity, to search for structures and ideas.

Find a better way to collaborate

In 3decision, structural biologists, medicinal chemists and modelers share a common ground where they can test and connect their ideas.



Molecular Modeller

- ◇ Get an overview of all structural knowledge on your target (public and proprietary data)
- ◇ Find similar ligand-protein interactions in other protein families or projects
- ◇ Identify off-targets and new ideas through large-scale pocket similarity search
- ◇ Assess docking poses based on protein-ligand interaction statistics
- ◇ Generate ideas on how to modify your compound to increase the selectivity
- ◇ Share 3D views and highlighted results the way you see them

The Team

- ◇ Use 3decision as a common playground for analysis and ideation
- ◇ Organize structures, models and ligand collections in projects
- ◇ Find and reuse ideas created in other projects and research programs
- ◇ Export analyses and data to common data formats
- ◇ Integrate 3decision into your IT ecosystem via flexible REST APIs

Medicinal Chemist

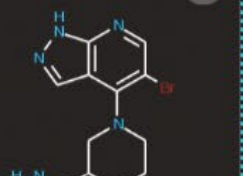
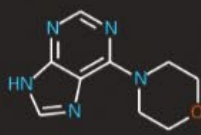
- ◇ Modify and redock a co-crystallized ligand
- ◇ Superpose two binding sites in one click
- ◇ Retrieve all compounds that are bound to your target
- ◇ Gather a list of compounds that bind to similar binding pockets
- ◇ Search for compounds that bind with similar interactions
- ◇ Share your design ideas with the project team

Structural Biologist

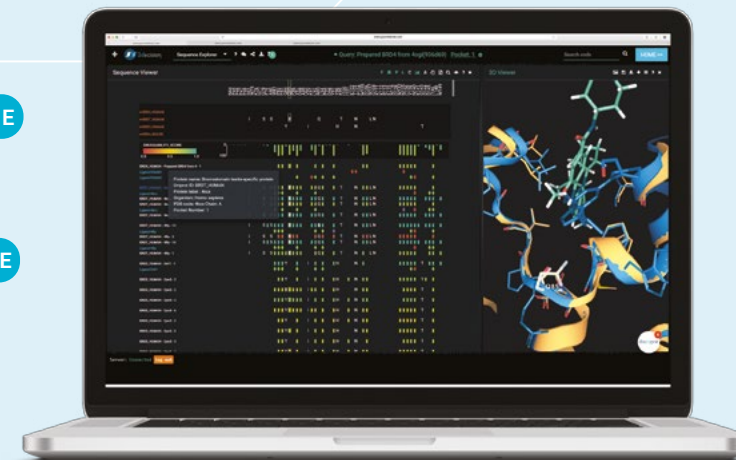
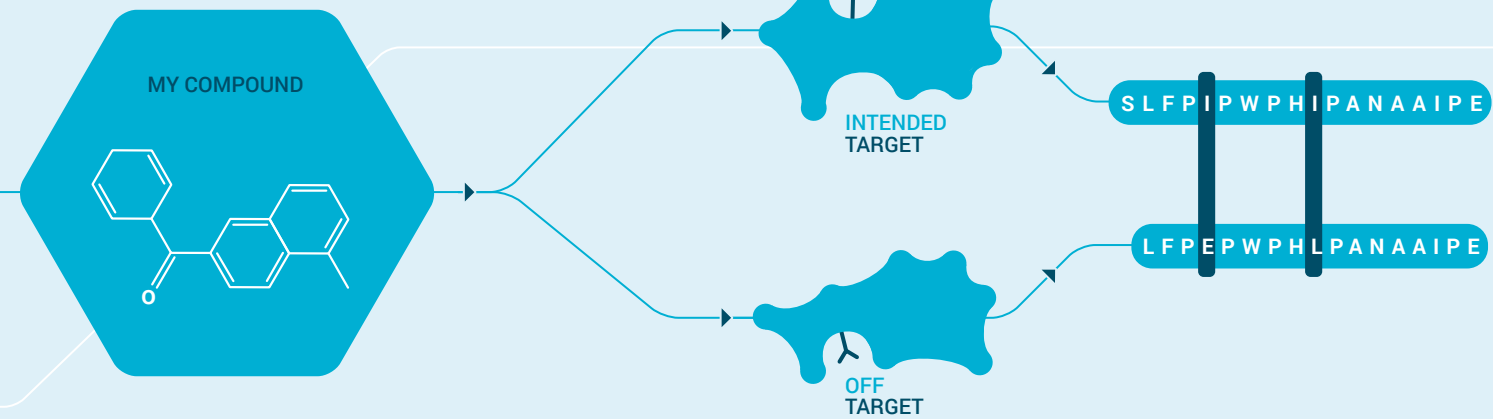
- Centralize and standardize ◇ the storage of structural data and associated files
- Share intermediate states of ◇ a resolved structure before publishing the final version
- Associate PDF reports to ◇ a structure and share them with the project team
- Visualize electron density maps ◇
- Compare your structure to ◇ large-scale protein-ligand interaction statistics

XEZ

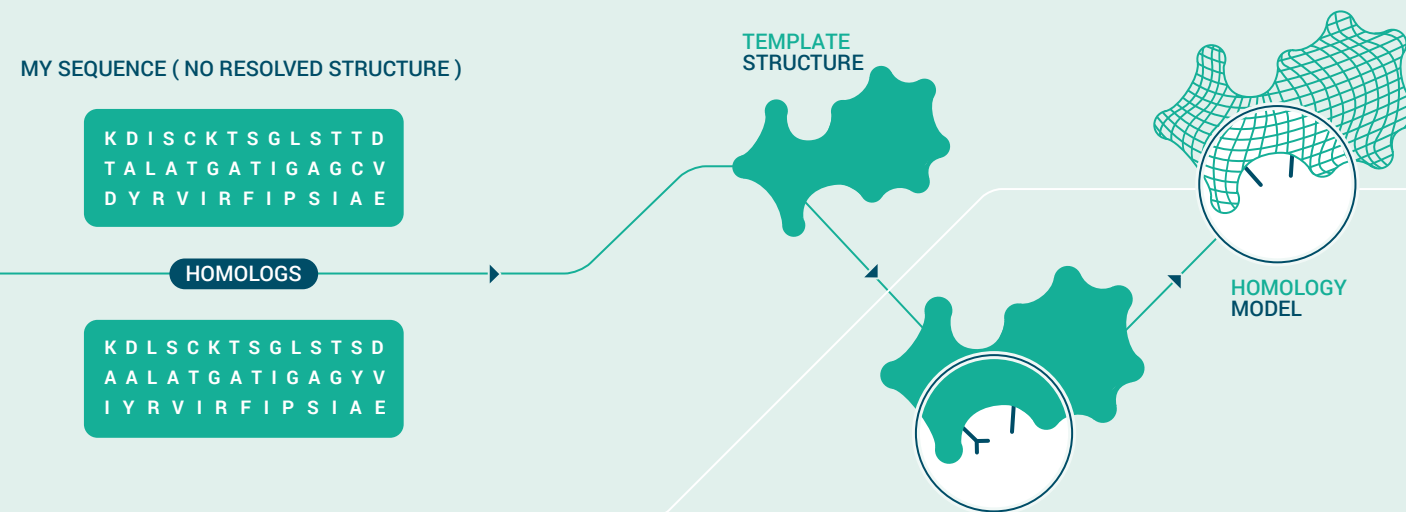
4UB



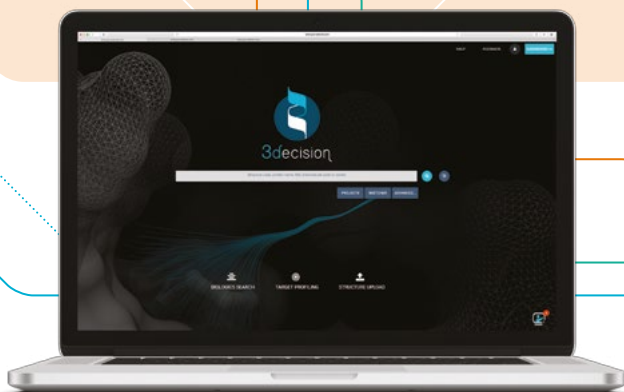
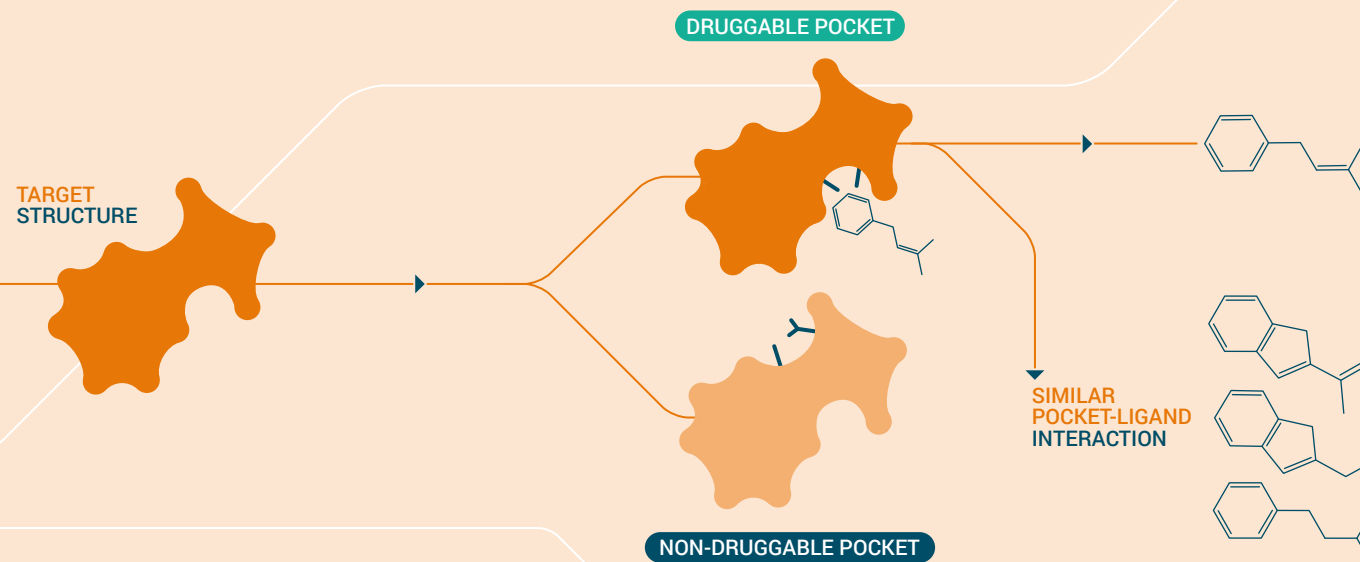
What can boost the selectivity of my compound?



What does my binding site look like?



What compounds bind to my target?



NAVIGATE THE BIOMOLECULAR DATA LANDSCAPE

3 offers to meet your needs



3decision Enterprise

Safely access, visualize and exploit your structural data.

PRIVATE SERVER SETUP | PER USER PRICING



3decision Community

Simplify the collaboration and sharing of structural knowledge.

COMMUNITY CLOUD | MONTHLY SUBSCRIPTION



Reports & Services

Get customized access to the 3decision technology.
Choose between a standardized report and a tailor-made consulting service.

ON DEMAND REPORT

CUSTOMIZED SERVICE

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