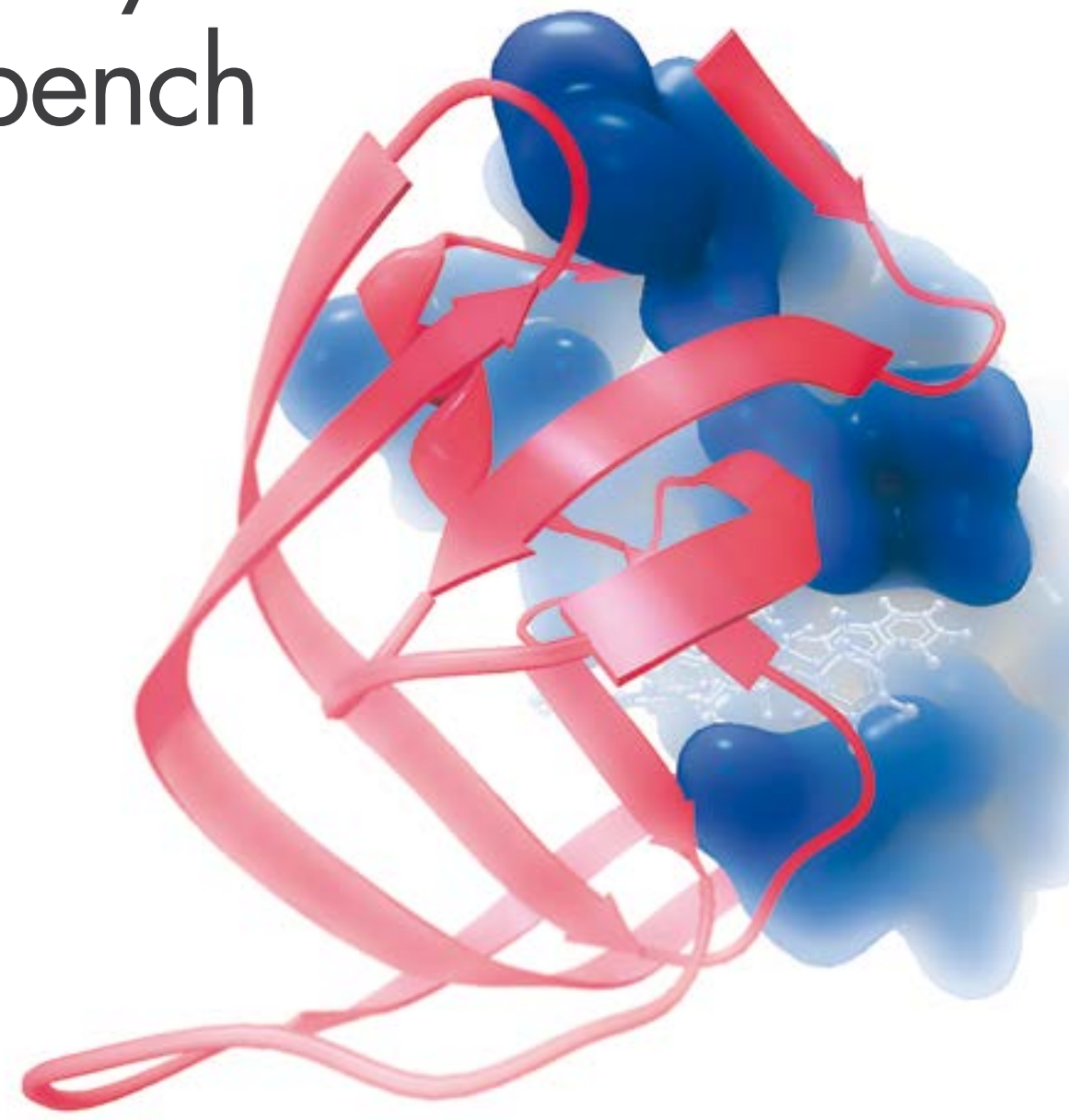
QIAGEN

CLC Drug Discovery Workbench



Sample to Insight

Molecule Structure Visualization

- Molecule 3D structure import: Mol2, SDF, PDB
- Direct download of PDB structures from NCBI
- Quick-style options including ball-n-sticks and molecular surfaces
- Custom visualization applied to selected atoms
- Save molecule visualizations on data
- Molecule tables with 2D depiction of molecules

Chemical Awareness

- Generate molecule 3D structure from SMILES or 2D representation*
- Automatic assignment of atom and bond properties
- Automatic binding site setup
- Chemical consistency check
- Lipinski's rule of five check

Structure Based Drug Discovery

- Binding pocket finder
- Easy, graphical protein target setup
- Fast track molecular docking
- Optimize ligand interactions in binding site
- Virtual screening
- Repair or change amino acids
- Calculate molecular properties
- Protein structure and binding site alignment

Sequence Analysis and Modeling

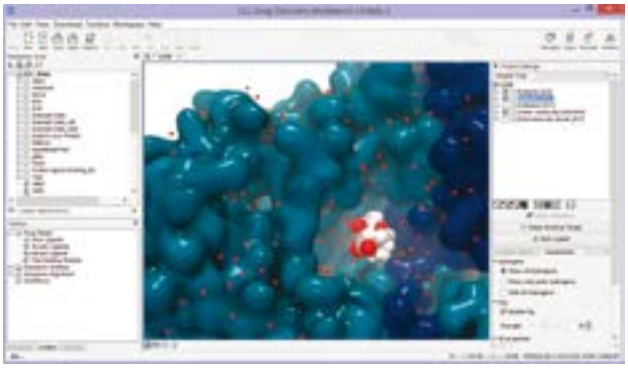
- Search for sequences at UniProt
- Create protein structure homology model
- BLAST
- Sequence alignment and phylogenetic trees
- Motif and Pfam domain search

* The freely available program Balloon is used as an engine for generating 3D coordinates for the molecule on import.

A Virtual Lab Bench for Chemists

CLC Drug Discovery Workbench is your new virtual lab bench. It gives you access to atomic level insights in protein-ligand interaction, and allows new ideas for improved binders to be quickly tested and visualized.

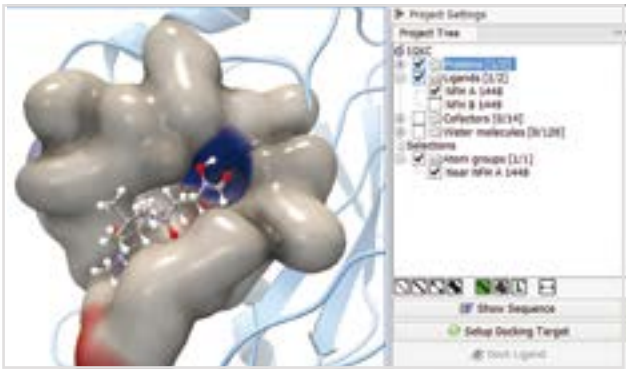
The workbench empowers bench chemists as well as computational chemists to analyze and visualize protein targets and ligands binding to them. The intuitive and powerful interface is designed to communicate with all chemists, regardless of their background in computational chemistry. Medicinal chemists can visualize and model molecule interactions to work with ideas in a frictionless manner, thus fueling innovation. CLC Drug Discovery Workbench is part of the CLC bio Enterprise Platform with support for workflows, client-server setup, and command-line tools. Furthermore, like all other workbenches from CLC bio, the Drug Discovery Workbench runs on Mac OS X, Windows, and Linux platforms.



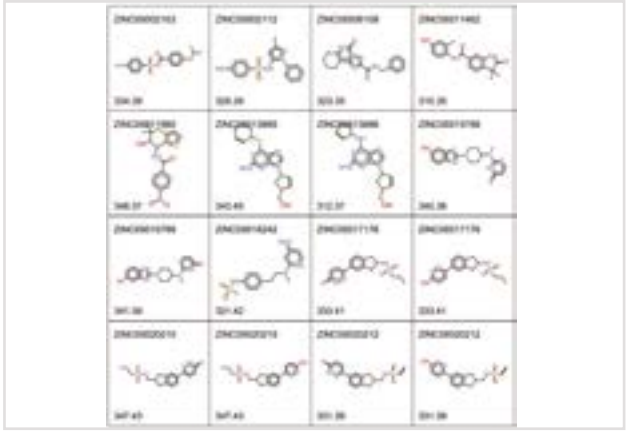
The interface of CLC Drug Discovery Workbench

Molecule Structure Visualization

It is fast and intuitive to customize the visualization of molecules in CLC Drug Discovery Workbench. The molecules are automatically sorted in categories: proteins, nucleic acids, ligands, cofactors, and water molecules. A selection of visualization styles is readily accessible via quick-style buttons. Custom atom groups can easily be created, and individual visualization styles can be specified for the group.



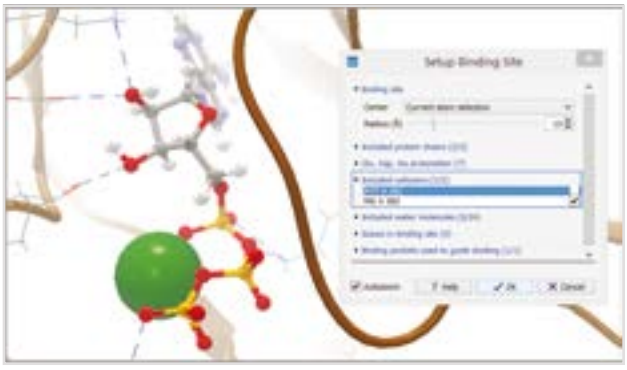
Project tree with quick-style buttons



Print 2D depictions from Molecule Tables in grid layout

Chemical Awareness

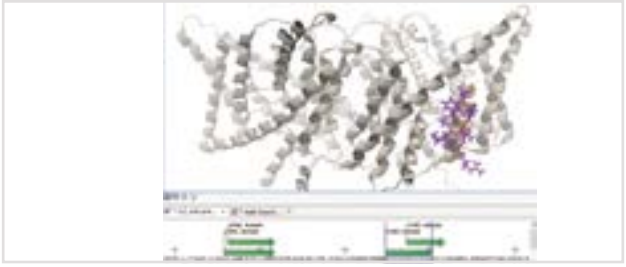
CLC Drug Discovery Workbench turns atom coordinates into chemical structures. A SMILES string can be copied from a 2D molecule sketching program, such as MarvinSketch or ChemDraw, and pasted directly into the Workbench. All molecules are continuously checked for chemical consistency, such as correspondence between atom hybridization and bond pattern. A target protein is automatically set up for docking by a one-click option and an interactive guide is provided to inspect and adjust the setup.



Interactive guide to inspect and adjust binding site setup

Sequence Analysis and Modeling

Protein structure homology models can be created in two easy steps. Sequence alignments can be linked to a protein structure, to study consequences of variation in a 3D context. Sequences can be annotated, and annotations can be transferred between sequence and structure.

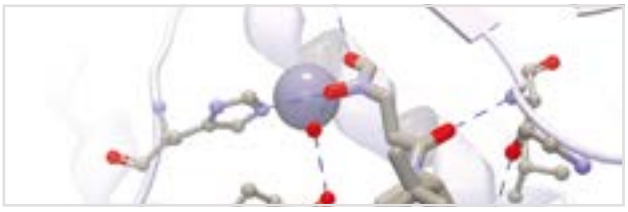


Sequence annotation transferred to protein structure

Structure Based Drug Discovery

Ligands can be docked with one click in the graphical user interface, or through a wizard, allowing customization of sampling and output. Huge molecule libraries are handled

in Molecule Tables for use in virtual screenings. Ligands can be modified directly in the binding site to optimize protein interaction. The binding modes of ligands, being co-crystallized or resulting from docking, can be inspected in detail using automatically generated visualizations of the interactions between ligand and docking target.



Ligand binding inspection

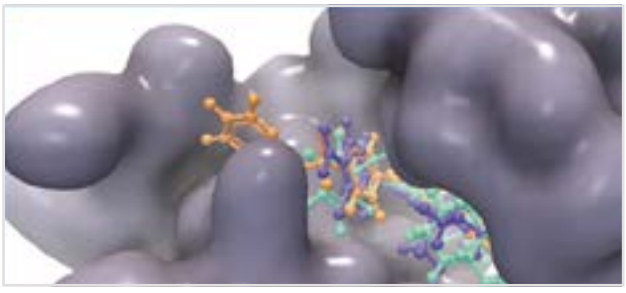
Program	Company	Result
CLC Drug Discovery Workbench	CLC bio	83%
Glide SP **	Schrodinger	82%
MOE **	CCG	80%
Molegro Virtual Docker	CLC bio	80%
AutoDock ***	Scripps Research Inst.	78%
FlexX-HYDE ***	BioSolveIT	75%
FRED**	OpenEye	70%

* J. Med. Chem. 50 (2007) 726-741

** J. Comput. Aided Mol. Des. 26 (2012)

*** J. Med. Chem. 55 (2012) 623-638

Binding site visualized while optimizing ligand



Three docking results shown in different colors and with docking target shown as molecular surface

Accuracy Benchmark

For a diverse set of 85 high resolution protein-ligand complexes* relevant to the pharmaceutical or agrochemical industry, the table shows how many complexes are correctly predicted by the top ranked docking result (RMSD less than 2.0 Å).

Discover more and download trial at: **www.clcbio.com/DrugDiscovery**

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