CLC **Drug Discovery** Workbench

FEATURES AND BENEFITS

MOLECULE STRUCTURE VISUALIZATION

- Molecule 3D structure import: Mol2, SDF, PDB
- Search for PDB structures at NCBI
- Molecule 3D structure export: Mol2
- Quick-style options including ball-n-sticks and molecular surfaces
- Custom visualization applied to selected atoms
- Molecule tables with 2D depiction of molecules

CHEMICAL AWARENESS

- Molecule 3D structure generation from SMILES or 2D representation*
- Automatic assignment of missing atom and bond properties
- Automatic docking target setup
- Chemical consistency checker

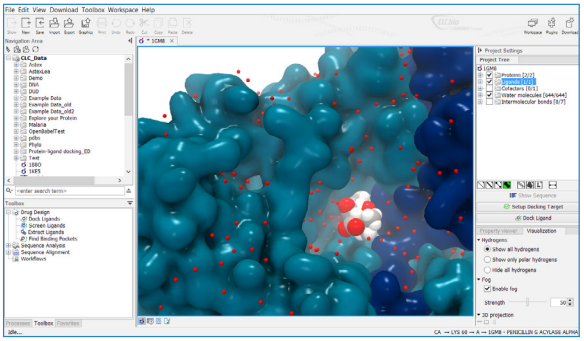
STRUCTURE BASED DRUG DISCOVERY

- Manually adjust atom and bond properties
- Binding pocket finder
- Easy, graphical docking target setup
- Fast track molecular docking
- Virtual screening
- Size of molecule libraries not limited by memory
- Ligand binding inspection

SEQUENCE ANALYSIS TOOLS

- Search for sequences at UniProt
- BLAST
- Alignments
- Phylogenetic trees
- Prediction of transmembrane helices
- Motif search
- 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

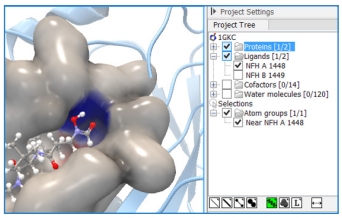
CLC Drug Discovery Workbench is your new virtual lab bench. It gives you access to atomic level insights in protein-ligand interaction, and allows new ideas for improved binders to be quickly tested and visualized.

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, with no assumptions about their level of theoretical training. Medicinal chemists can visualize and model molecule interactions to work with ideas in a frictionless manner, thus fueling innovation.

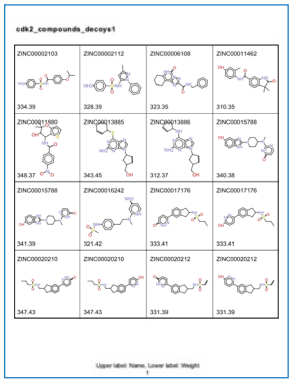
CLC Drug Discovery Workbench is part of the CLC bio Enterprise Platform with support for workflows, client-server setup, and command-line tools. Furthermore, like all other workbenches from CLC bio, the Drug Discovery Workbench runs on Mac OS X, Windows, and Linux platforms.

Molecule Structure Visualization Features

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



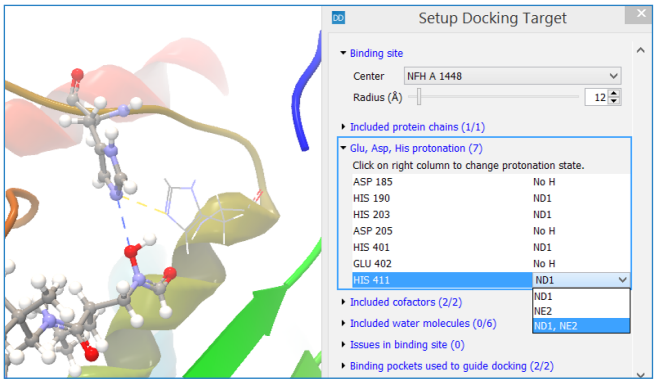
Project tree with quick-style buttons



Print 2D depictions from Molecule Tables in grid layout

Chemical Awareness

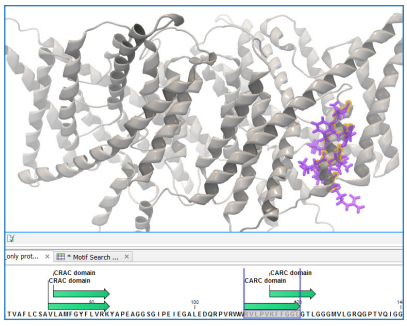
CLC Drug Discovery Workbench turns atom coordinates into chemical structures. A SMILES string can be copied from a 2D molecule sketching program, such as MarvinSketch or ChemDraw, and pasted directly into the Drug Discovery Workbench. All molecules are continuously checked for chemical consistency, such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



Interactive guide to inspect and adjust the automatic docking target setup

Sequence Analysis and Alignment

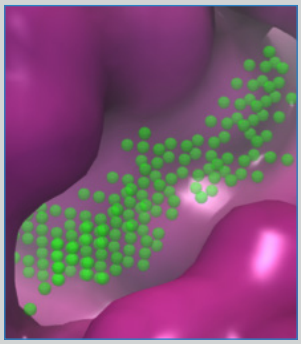
Homologous proteins can be found and compared using the built-in BLAST search and alignment tools. Phylogenetic trees can be generated, to show the relationship between sequences. Sequences can be annotated with functional information using tools for motif and Pfam domain search.



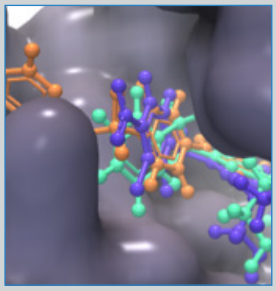
Cholesterol binding motifs (CRAC and CARC) found on a chloride channel

Structure Based Drug Discovery Features

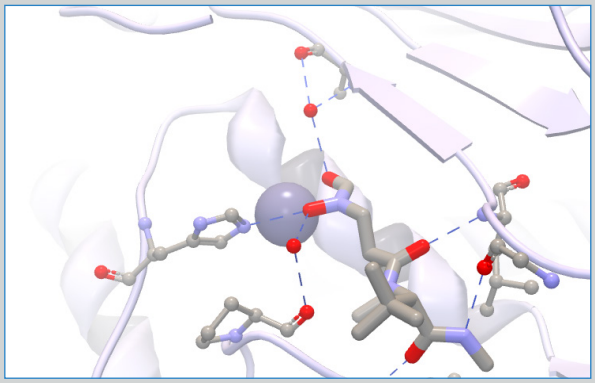
Ligands can be docked with one click in the graphical user interface, or through a wizard, allowing customization of sampling and output. Huge molecule libraries are handled in Molecule Tables for use in virtual screenings. Potential ligand binding sites can be located with the binding pocket finder. 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.



Finding potential binding pockets



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



Ligand binding inspection

Accuracy Benchmark

For a diverse set of 85 high resolution protein-ligand complexes* relevant to the pharmaceutical or agrochemical industry, it is tested how many of the complexes can be reproduced in molecular docking with a ligand binding mode with RMSD of less than 2 Å.

Program	Company	Result
CLC Drug Discovery Workbench	**CLC bio**	**83%**
Glide SP**	Schrödinger	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

CLC bio · EMEA
Silkeborgvej 2 · Prismet
8000 Aarhus C
Denmark
Phone: +45 7022 5509

CLC bio · Americas
10 Rogers St # 101
Cambridge · MA 02142
USA
Phone: +1 (617) 945 0178

CLC bio · AsiaPac
69 · Lane 77 · Xin Ai Road · 7th fl.
Neihu District · Taipei · Taiwan 114
Taiwan
Phone: +886 2 2790 0799

CLC bio
A QIAGEN® Company