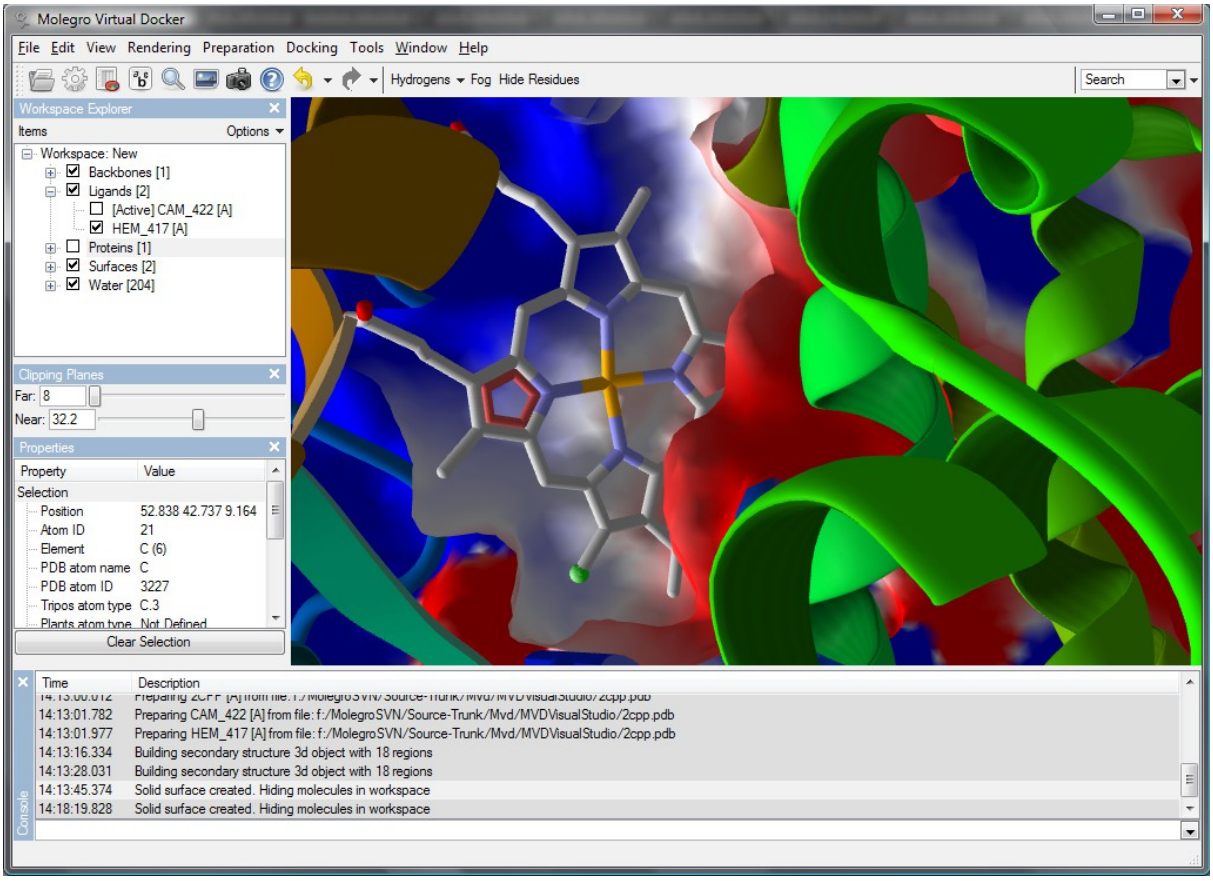
Molegro Virtual Docker

High accuracy molecular docking

Computational methods are now a ubiquitous part of modern drug design. Being able to predict and visualize drug candidates and their interactions with the target receptor makes it possible to understand and rationally optimize potential drugs - an important advantage in a competitive billion-dollar industry.

Molegro Virtual Docker offers the easiest and most accurate way to predict how molecules interact with proteins in a fully integrated environment.

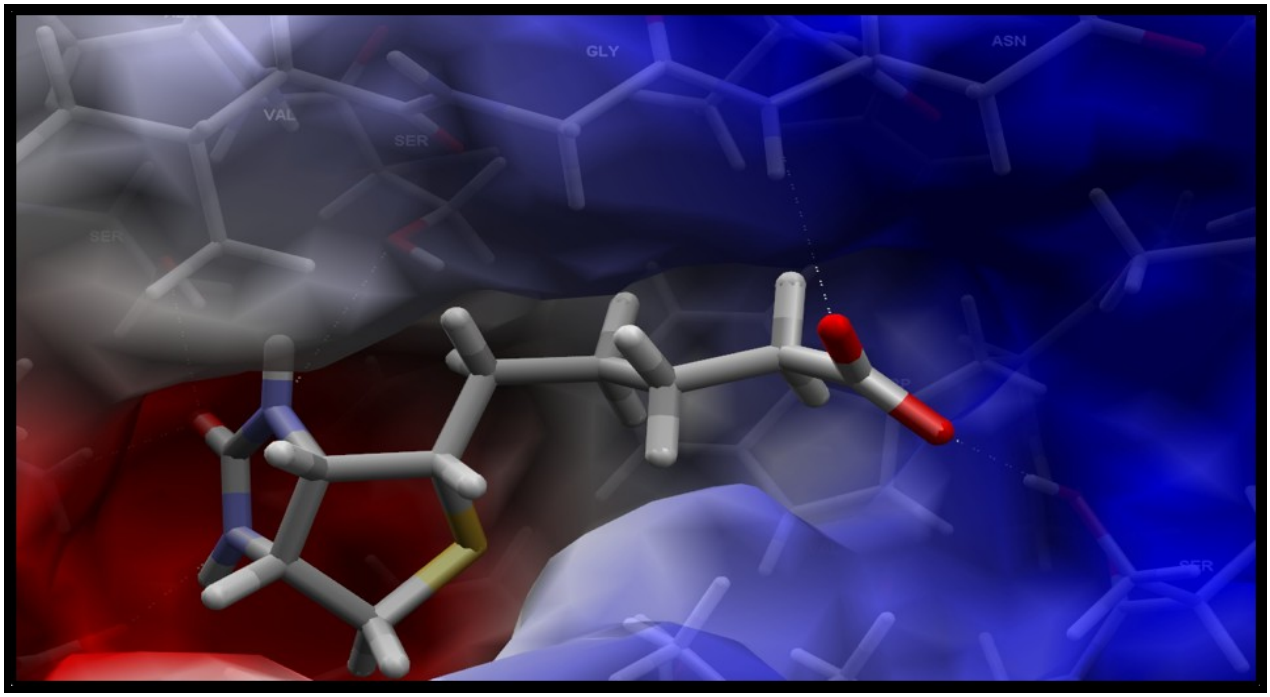


- Predict and analyze protein-ligand interactions
- Screen compound databases for activity against a receptor
- Determine molecule similarity
- Build regression models based on structural information
- Distribute and script calculations
- User-friendly interface with intuitive wizards

Protein-Ligand Docking

Predict how small flexible molecules interact with a protein receptor.
Screen databases for potential drug candidates or refine existing leads.

- Predict potential binding sites
- Protein binding pocket flexibility
- Visually inspect docking predictions with relevant interactions
- Repair, mutate, or minimize sidechains before docking
- Displaceable water model
- Import and export of industry standard file formats (PDB, Mol2, SDF)
- Automated preparation of input structures



Benchmark Results

Our software provides very accurate predictions of ligand binding modes.
It has been cited in more than 1200 research papers, and is used by organizations across the world. See molexus.io for a list of references.

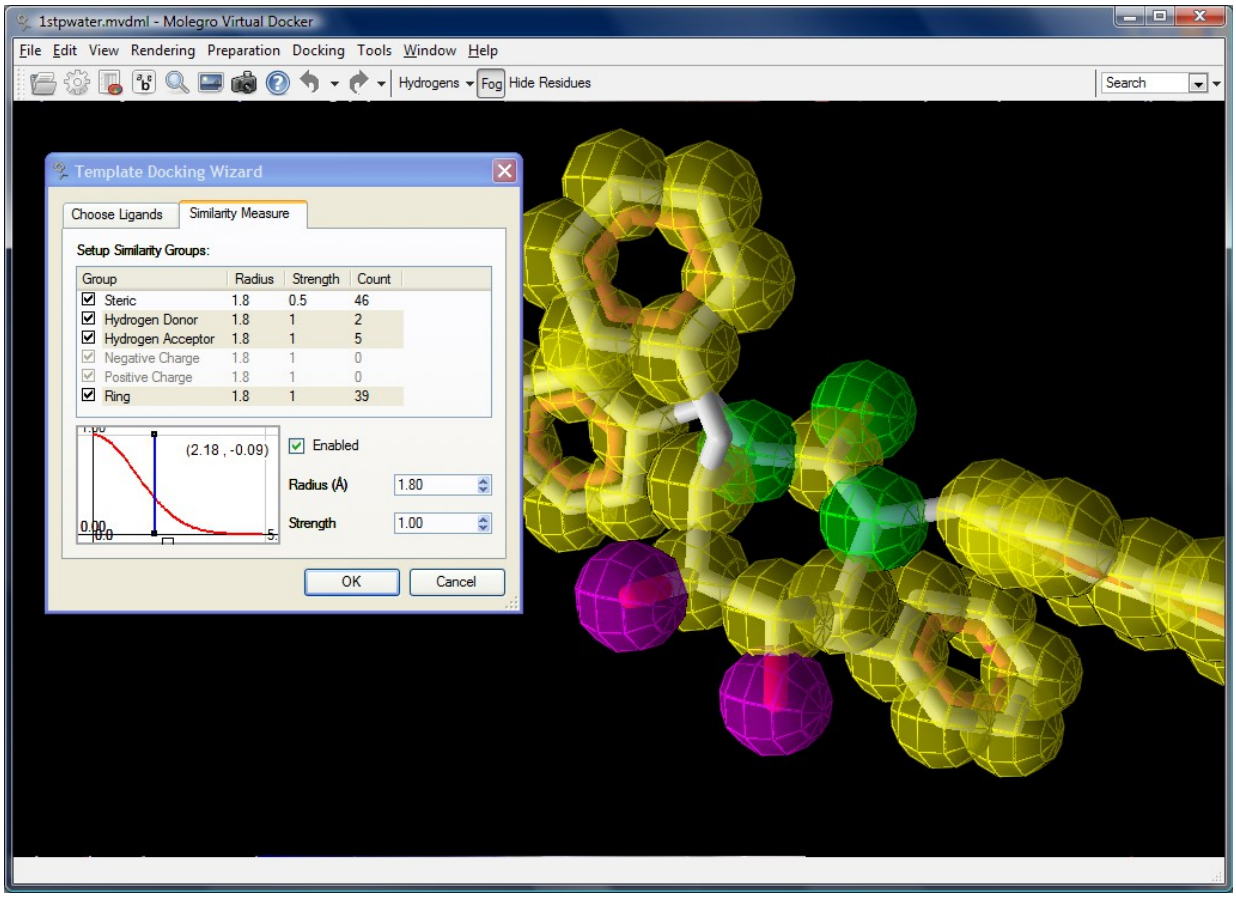
Docking Program	Accuracy
Molegro Virtual Docker	**87.0%**
Glide	81.8%
GOLD	78.2%
Surflex	75.3%
FlexX	57.9%

Results from '*MolDock: A New Technique for High-Accuracy Molecular Docking*' (J. Med. Chem., 2006, 49(11), pp 3315 – 3321).

Ligand-Based Drug Discovery

Don't know the protein structure? Molegro Virtual Docker makes it possible to screen databases based on structural and chemical similarity with known binders. You can also perform flexible molecule alignment, or create advanced regression models based on chemical features.

- Flexible ligand alignment
- Screen databases for similarity with known binders
- Molecular descriptor calculation, including our unique 2D CFDM topological descriptors for building QSAR models
- Extract 3D molecule descriptors based on chemical properties
- Finetune scoring based on shape or chemically relevant features

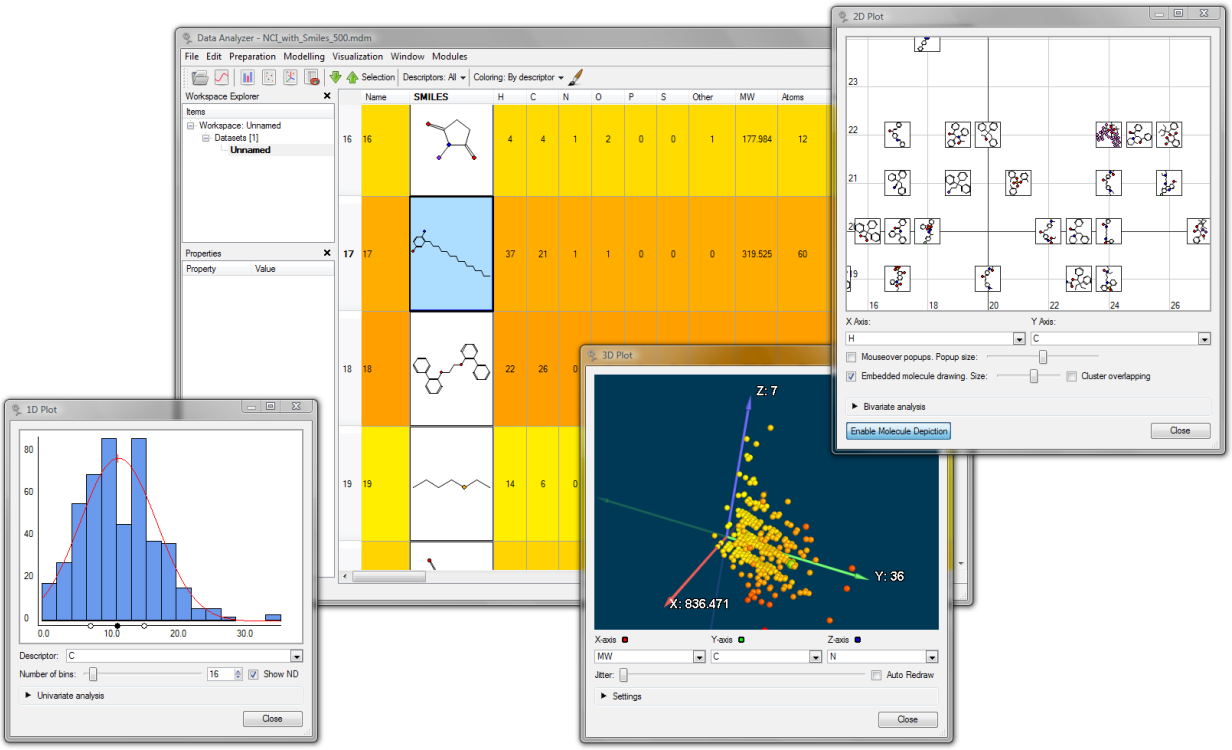


Hybrid Docking: Combining Ligand and Receptor Knowledge

If you have structural knowledge about how existing ligands bind to a receptor, there is no need to throw information away. Molegro Virtual Docker makes it possible to dock into the receptor and a template generated by a ligand simultaneously.

Integration and Analysis

- Built-in tools for advanced data analysis and visualization using Molegro Data Modeller (bundled with Molegro Virtual Docker)
- Workflow support through KNIME makes it easy to connect to third-party software and databases
- Script from the command-line or using Python



Built-in data analysis and visualization

Supported Windows Platforms

- Windows 10
- Windows 8 / 8.1
- Windows 7

Evaluation Copies

- To try a free 30 day trial license visit www.molexus.io/trial.php

Additional Information

- www.molexus.io
- sales@molexus.io

molexus

Molexus develops cheminformatics software for drug discovery and data mining.

We focus on combining state-of-the-art algorithms with an intuitive graphical user interface experience.

Through collaboration with both academia and industry we ensure our products are continuously evolving.

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