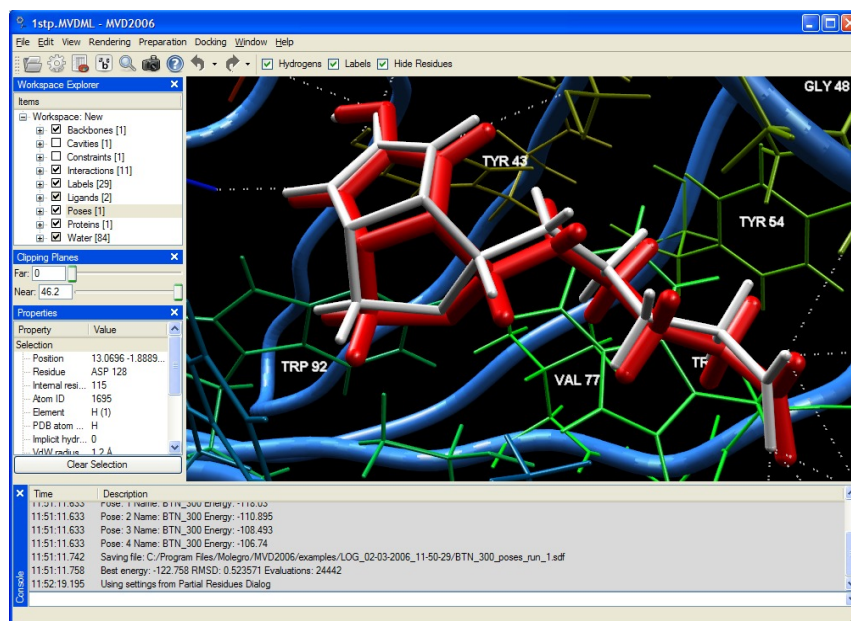


Molegro Virtual Docker 2006

High accuracy molecular docking

Molegro Virtual Docker is an integrated platform for predicting protein - ligand interactions. It handles all aspects of the process, from preparing the molecules to determining the potential binding site of the target protein and predicting the binding mode of the ligand.

Molegro Virtual Docker offers high-quality docking based on a novel optimization technique combined with a user interface experience focusing on usability and productivity.



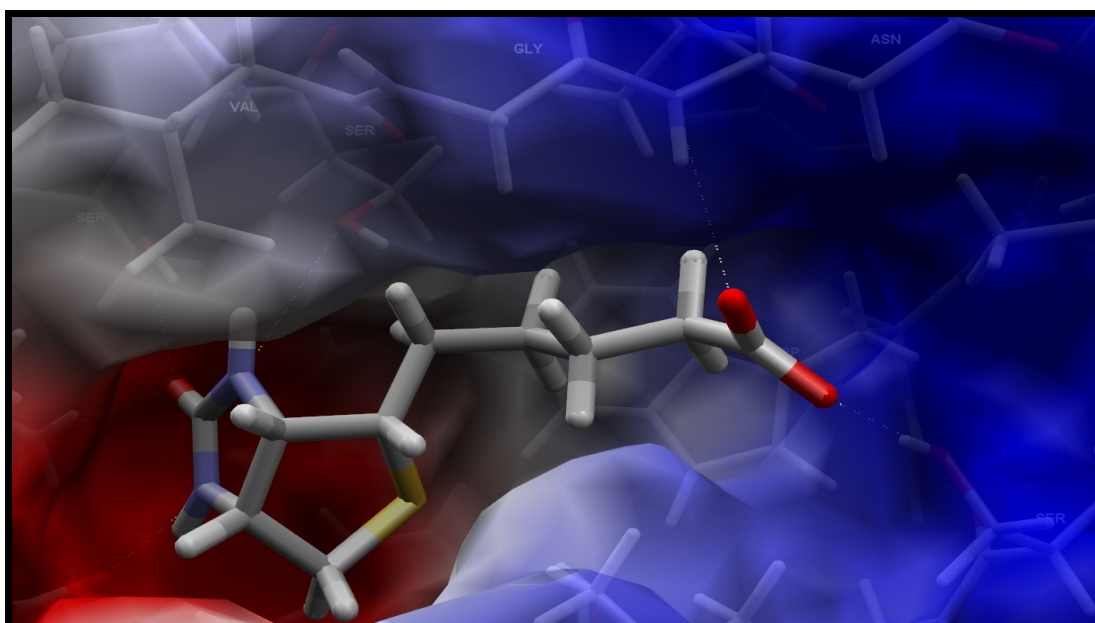
The main workspace window of Molegro Virtual Docker.

Molegro Virtual Docker Provides

- **High docking accuracy:** the docking engine has been proven to correctly identify binding modes with high accuracy. On the benchmark set listed in Table 1, Molegro Virtual Docker is shown to outperform other docking programs with regard to identification of correct binding modes.
- **Easy-to-use interface:** the built-in wizards enable the user to easily setup and perform docking runs. Advanced visualization and analysis tools are provided to examine ligand-receptor interactions and fine-tune found docking solutions.
- **Cross-platform:** supported on Linux, Windows and Mac, allowing easy interoperability between platforms.

Basic Features

- Import and export of industry standard file formats (PDB, Mol2, SDF)
- Automated preparation of input structures (assign hydrogens, charges, bond orders, hybridization)
- Visualization styles (wireframe, ball-and-stick, CPK, stick, surfaces)
- Automatic prediction of potential binding sites (active site finding)
- Flexible 3D-label system
- Docking scoring function (extended PLP score taking hydrogen bonding directionality and solvation into account)
- Docking search algorithm based on state-of-the-art genetic algorithms
- Console command interface to allow for advanced user interaction
- GUI wizards and on-line help



A docking pose highlighting relevant interactions

Benchmark Results

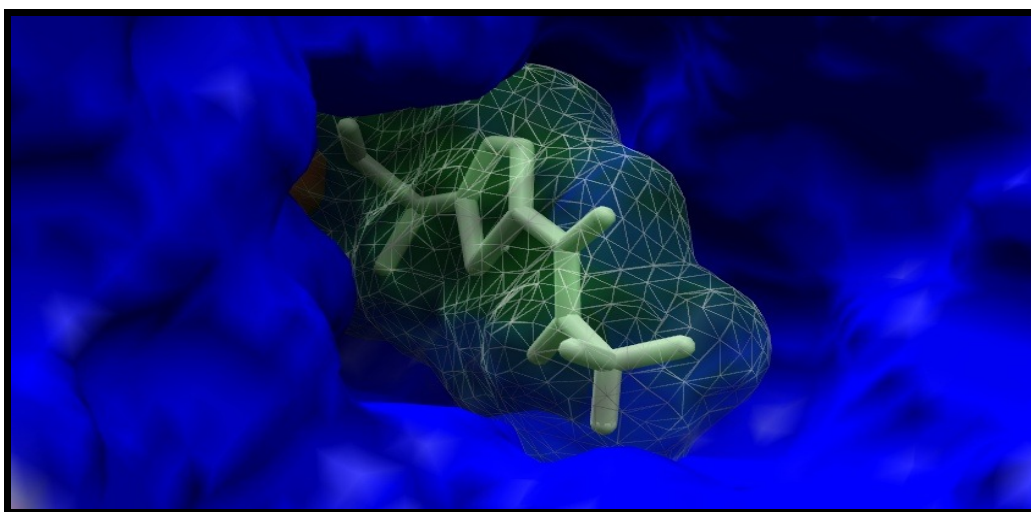
Docking Program	Surflex77 Accuracy
Molegro Virtual Docker	87.0%
Glide	81.8%
Surflex	75.3%
FlexX[*]	57.9%

Table 1: Accuracy of selected docking programs. A binding mode is regarded as correctly identified if the RMSD (to the native co-crystallized ligand) is less than 2.0Å. Before docking the ligands were energy minimized and randomized and all water molecules were removed from the complex. The dataset consists of the 77 complexes from the Surflex set as defined in *Friesner et al.*: 'Glide: A new approach...' *J. Med. Chem.*, Vol. 47, pp. 1739–1749, 2004.

[*] Based on 76 out of the 77 complexes in the Surflex77 set.

Advanced Features

- Visual inspection of docked conformations displaying relevant interactions
- Manual/semi-automated modification of docked conformations
- Realtime visualization of the docking process (e.g. found poses, energy plots)
- Ability to only report diverse conformations based on a clustering measure
- Reranking score (rerank docked solutions to increase docking accuracy)
- Estimation of binding affinity
- Customizable scoring function (alter scoring function by manually setting coefficients and selecting which energy terms to include)
- The user interface can be customized and extended via the built-in macro language
- User-defined constraints to increase docking performance



System Requirements

- Windows 2000, XP or 2003
- Mac OS X 10.4.x
- Linux: Most standard distributions (RedHat, Fedora Core, ...)
- Other platforms are supported on demand

Evaluation Copies

- To request a 30 day trial version contact evaluation@molegro.com.

Additional Information

- www.molegro.com
- info@molegro.com

About Molegro

The name 'Molegro' is a combination of the words 'Molecule' and 'Allegro' (Italian for rapid). The core of our business is high-performance drug discovery solutions leading to a faster drug-development process.

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