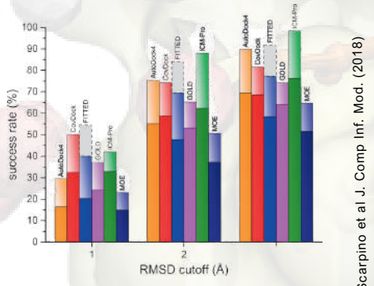
ABOUT MOLSOFT

Founded in **1994** in San Diego, USA, Molsoft is a leading provider of software tools and consulting services in the area of **structure prediction, structural proteomics, rational drug design, bioinformatics and cheminformatics**.

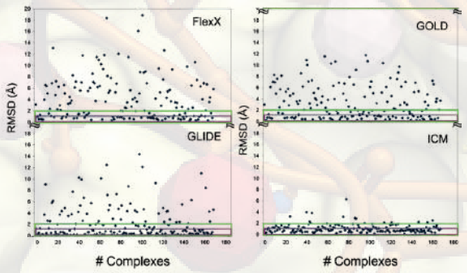
More than **6,500 citations** in Google Scholar with more than **1000 publications** in peer- reviewed journals.

List of Publications



Scarpino et al J. Comp Inf. Mod. (2018)

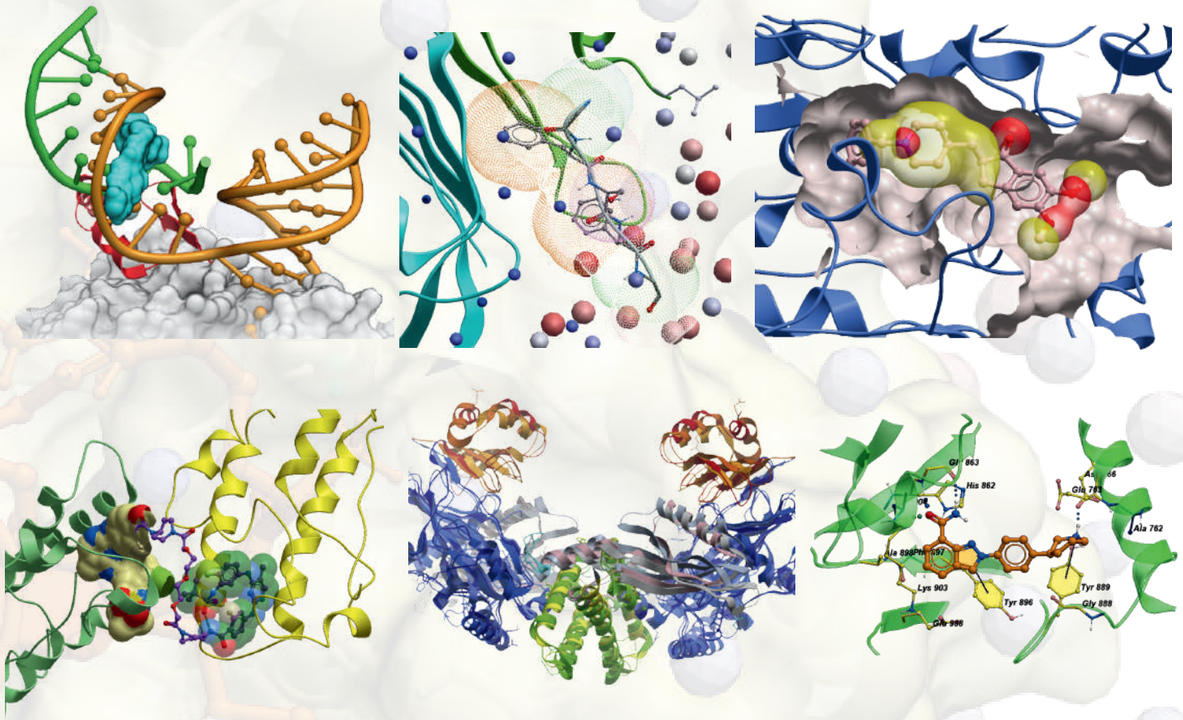
ICM Pro outperformed other programs in covalent docking



Hongming Chen at al. Astrazenica R&D, J. Comp Inf. Mod. (2006)

On Evaluating Molecular-Docking Methods for Pose Prediction and Enrichment Factors

Other comparative studies



ABOUT ADVENT

Advent Informatics was founded in 2016 in Pune. Advent focuses on providing well-renowned software to Indian researchers. We also represent the following companies:

Chemaxon

Chemoinformatics, Chemical structure storage & search, Library Enumeration, property prediction

ChemPass

AI-Assisted Lead Discovery and Forward reaction-based design using rule-based AI

keymodule

Optical Structure Recognition tool for extracting chemical structures from documents & images.

CERTARA

D360: Scientific informatics system for small molecule and biologics discovery research.

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ADVENT INFORMATICS PVT LTD

MOLSOFT

A COMPREHENSIVE PLATFORM FOR MOLECULAR MODELING & DRUG DISCOVERY

MolSoft's ICM software is built on the Internal Coordinates (IC) representation, which naturally captures the bond geometry and flexibility of molecules. This enables efficient and accurate conformational modeling. ICM uses the Biased Probability Monte Carlo (BPMC) method for powerful global optimization, making it well-suited for a wide range of molecular modeling and computational chemistry applications.

www.adventinformatics.com/molsoft/
www.molsoft.com/

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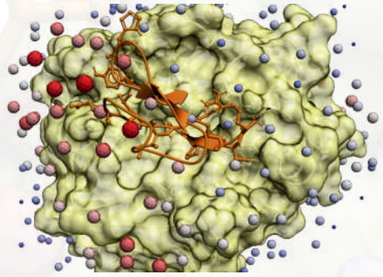
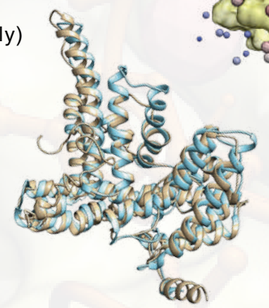
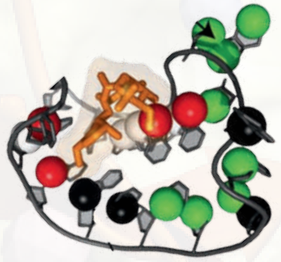
ICM-PRO DESKTOP MODELING

ICM-Pro is MolSoft's primary desktop modeling software offering the most of the core functionalities



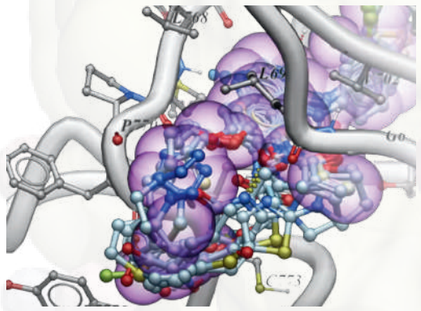
- ICM Pocket Finder
- Protein Structure Modeling and Analysis
- Small Molecule Docking (Upto 100 Compounds)
- 2D ligand-receptor interaction diagrams
- Protein-Protein/RNA Docking
- Peptide Docking and Screening
- ICM 3D Interactive Editor (docking Only)
- Induced Fit Docking
- PROTAC Modeling
- Molecular Dynamics
- Predict Effect of Mutation
- Crystallographic Analysis Tool
- Sequence Analysis & Alignments
- Homology Modeling
- Loop Modeling



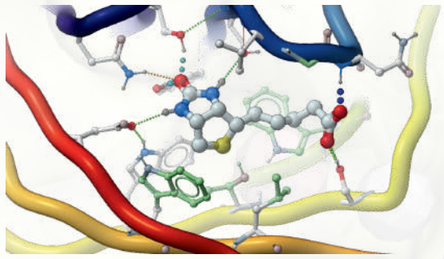


ICM-PRO VLS (VIRTUAL LIGAND SCREENING)

ICM Virtual Ligand Screening (VLS) allows you to undertake high throughput structure (Docking based) and Ligand (Pharmacophore) based virtual screening on a local server or cloud. Some commonly used features include:



- Ligand Docking - Batch
- Covalent Docking
- Structure-based VLS
- Virtual Ligand Screening Physics/AI based scores
- Ligand-based VLS (APF)
- Fragment-based VLS
- Dock on the fly Markush generated libraries
- ICM 3D Interactive Editor*
- Atomic Property Fields (APF)
- RIDE (CPU version)
- SAR analysis - MPA, SALI, Free Wilson Regression*



- Pharmacophore Searching
- Chemical and ADMET Properties *
- Multi-Parameter Optimization*
- Hierarchical Chemical Clustering*
- 2D and 3D QSAR*
- Combinatorial Chemistry*
- Conformer Generation*
- Chemical Spreadsheet and Chemical Search*
- Chemical Superposition Tools*

*Also available in ICM Chemist Pro

Module wise feature comparison

FREE TOOLS

- ICM-Browser
- ActiveICM
- PDB Viewer
- 2D to 3D Chemical Converter
- Drug Likeness prediction.
- Interactive Torsion Profile Prediction.

LICENSE OPTIONS

- Floating or Node Locked
- 1, 3 and 5 Years

Free academic Teaching license available (contact us for details)

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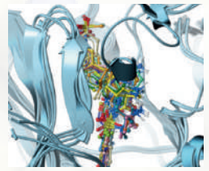
ULTRA LARGE LIBRARY HANDLING & VIRTUAL SCREENING /AI TOOLS

molsoft molecules in silico

RIDGE (RAPID DOCKING GPU ENGINE)

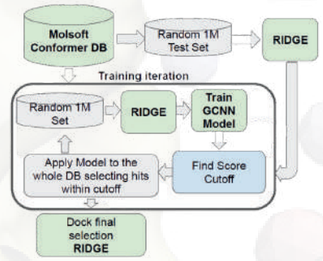
RIDGE is an Ultra-fast **Structure based Docking engine for giga sized libraries.**



- Key stages are fully GPU parallelized with Low-level CPU multithreading. Supports Multiple GPUs.
- **~100 compounds/sec docking speed** (using RTX 4090),
- Screen **10M compounds in less than 30 hours** on a single modern-day desktop

GIGA-SCREEN

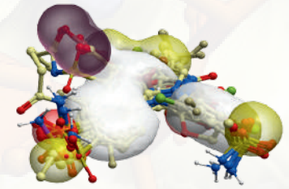
GigaScreen is a combination of **Machine Learning and Deep Learning tools applicable to very large chemical libraries.**



- The docking Engine can be RIDGE or Molsoft VLS
- Pose Scoring can be done using RTCCN or VLS
- Uses Machine Learning to build prediction models using docking scores and chemical structures
- Gigascreen of 1.9B compounds (Enamine REAL) takes around 3-4 days.

RIDE (RAPID ISOSTERE DISCOVERY ENGINE)

RIDE is a fast 3D molecular similarity search method based on APF. It uses 3D ligand superposition based on highly sensitive and accurate APF molecular alignment technology.



RIDE searches databases of compound conformers for molecules that are isosteric to the query.

Speed Benchmarking:
RIDE GPU ~ **1.5 M conformers/sec/GPU** (RTX 4090)
RIDE CPU ~ **6,000 conformers/ sec/CPU**

MOLSCREEN

MolScreen is a set of high-quality 2D and 3D **AI/ML models** for a broad range of pharmacology and toxicology targets. Approximately 2,500 models against 1,200 targets are available. MolScreen can be used for:

- Target / Lead Identification
- Profiling Multiple protein targets
- Drug-Repurposing

GINGER

GINGER (Graph Internal-coordinate **Neural-network** conformer Generator with Energy Refinement) is Molsoft's new cutting-edge software designed for lightning-fast high quality conformer library generation on GPUs.

Some Pre- Prepared Screening Libraries (Offered with RIDE GPU and RIDGE)

eMolecules
eMolecules Synple> 7T
eMolecules Screening ~27M

Enamine
Enamine REAL ~5.6B
Enamine MADE BBs ~ 556M
Enamine REAL Diverse ~18M

WuXi AppTec
Wuxi Galaxi ~2.5B

mcule
MCULE ~40M

MolPort
Molport ~3.6 M

SAVI
SAVI Synthesizable ~1B

CHEM-SPACE
Chemspace Freedom Spcae ~160M

OTHER AVAILABLE MODULES

ICM Bio, ICM Chemist, ICM Chemist Pro, ICM Scarab, Molcart, GigaSearch

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