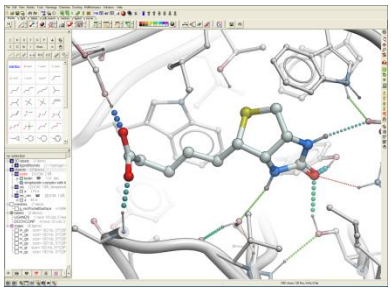
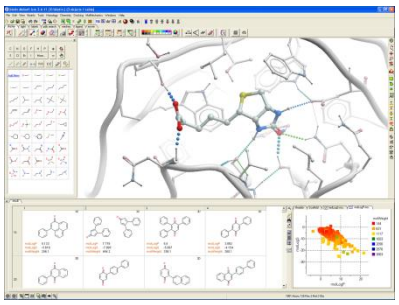
ICM Chemist Pro

For:
Win/Linux/Mac

Licensing:
- Annual
- Multi-Year
- Perpetual

License Type:
Single user machine or multi-user server.





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ICM Chemist Pro is a standalone cheminformatics products containing a wide set of 3D chemical tools, chemical superposition, 3D interactive ligand-receptor editing, and QSAR. **ICM Chemist Pro** contains the features described below as well as **all** the features contained within ICM Chemist and ICM-Browser-Pro.

Interactive Drug Design with the 3D ICM Ligand Editor The ICM Interactive 3D Ligand Editor is an easy-to-use desktop application that allows a chemist to visualize a receptor-ligand complex and then apply their experience and intuition to explore, design and optimize new drug-like compounds. Some key features include:
- Modify terminal atom with a chemical group.
- Fast building of heavy atom neighbors.
- Change atom properties and bond types
- Edit ligand in 2D molecular editor.
- Delete atoms and bonds.
- Display hydrogen bonds, binding pocket, and atomic energy circles.
- Add edited ligands to table and save.
- Convenient undo and redo feature.
- Dock and/or Minimize edited ligand.
- On the fly docking and scoring of replacement groups.
- Fragment-based docking and design.

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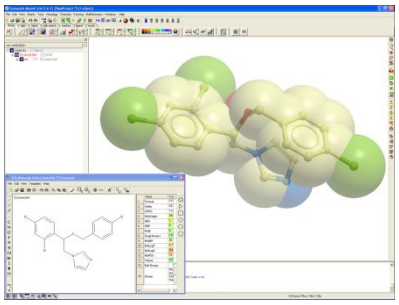

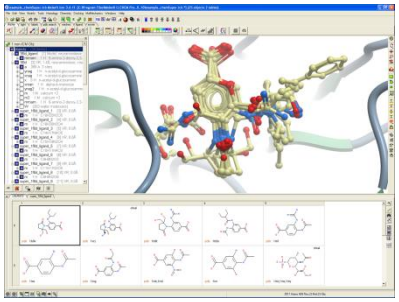

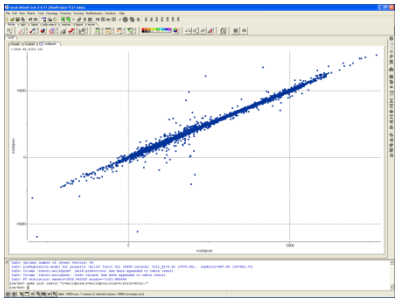

MolSoft LLC
3366 North Torrey Pines Court,
La Jolla, CA 92037
www.molsoft.com

E-Mail:
info@molsoft.com
Call:
+1 (858) 625-2000

MolSoft

Convert Chemicals to 3D.
Read in SMILES, MOL or SDF and convert to 3D. Browse chemicals in 3D directly from a chemical spreadsheet. All functions can be performed interactively or in batch mode.

Chemical Superposition Tools.
Rigid and flexible chemical substructure superposition. Atomic property field superposition (a 3D pharmacophoric potential). Tethered and directed superposition tools.

Quantitative Structure-Activity Relationship (QSAR).
Build and read prediction models. Various methods for linear and non-linear QSAR, machine learning tools for regression or classification, cross validation and boot strapping.

Plus all the ICM-Chemist 2D Tools as well.
- Draw and Edit Chemicals.
- Rich Environment for the Display and Manipulation of Chemical Datasets.
- Fast and Accurate Chemical Searching.
- Hierarchical Chemical Clustering and Trees.
- Generate Stereoisomers and Tautomers.
- Generate Combinatorial Chemical Libraries.