

# ICM-Chemist

## For:

Win/Linux/Mac

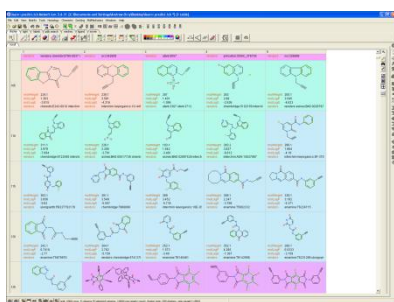
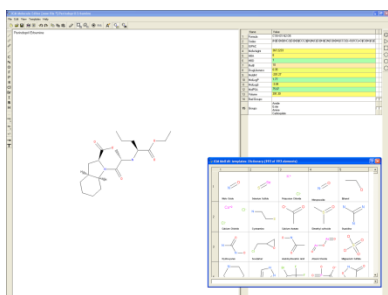


## Licensing:

Sold as perpetual license.

## License Type:

Single user machine or multi-user server.



**ICM Chemist** is a standalone suite of programs for chemical drawing and editing, chemical database generation, chemical searching, clustering, and enumeration. **ICM Chemist** contains the features described below as well as all the tools contained within **ICM Browser Pro**. For additional chemistry features including a wider set of 3D chemical options, chemical superposition, 3D interactive ligand-receptor editing, and QSAR please see **ICM Chemist Pro**.

## Drawing and Editing Compounds

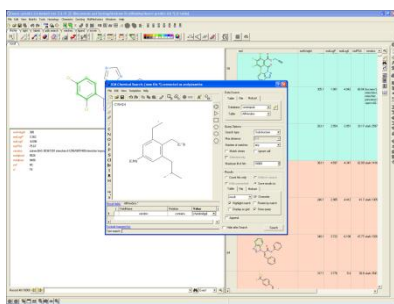
The ICM Molecular Editor is an easy-to-use chemical sketch pad for fast and accurate chemical drawing. As you sketch you can monitor the drug-like properties of your compound potentially toxic groups. A built in database of more than 1000 chemical templates is available to speed-up sketching.

## Rich Environment for the Display and Manipulation of Chemical Datasets.

Display and manipulate chemicals in spreadsheets, export in multiple formats including SDF and link directly to Microsoft Excel. Import new data columns and calculate new chemical property data on the fly. Compare multiple spreadsheets.

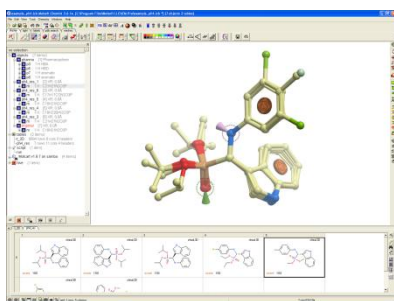


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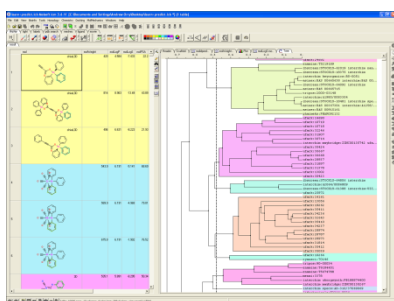
## Fast and Accurate Chemical Searching.

Search chemical databases using substructure, patterns, fingerprint similarity and exact match. Many customizable search rules and filter types are available. Search chemical spreadsheets or local databases. Output search results to new chemical spreadsheet or database.



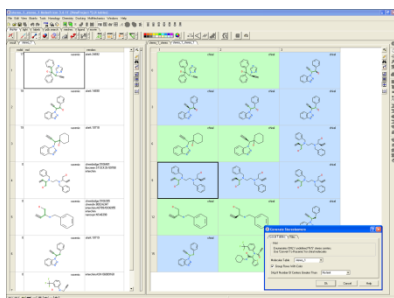
## 2D and 3D Pharmacophore Searching.

Sketch and edit 2D and 3D pharmacophores, search 2D and 3D compound database files, hits are scored and displayed in a chemical spreadsheet.



## Hierarchical Chemical Clustering and Trees.

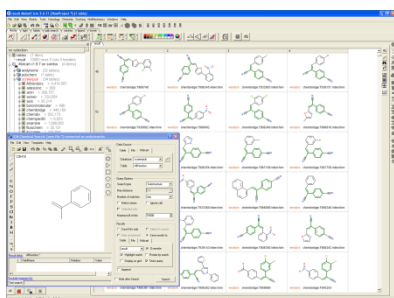
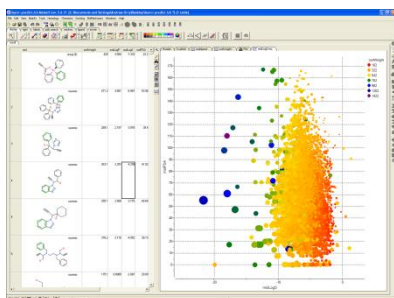
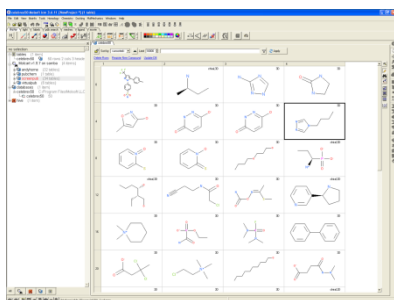
Cluster by Tamimoto distance as well as a variety of other data types. Fully interactive branch reordering and distance changing. Chemical spreadsheet is colored by branch and a representative "center" from each node can be selected.



## Generate Stereoisomers and Tautomers.

Generate stereoisomers and tautomers in batch mode or interactively from a table, mol or SDF file. Enumerate undefined R/S forms or convert to racemic for chiral forms.

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## **Store Large Chemical Libraries in Local Optimized Databases.**

Store millions of compounds in a fully optimized database for fast chemical search and other operations such as unique entry addition and diverse subset selection. Create databases from sdf, csv/tsv, SMILES and chemical spreadsheets, browse databases.

## **Display Chemical Data in Interactive Plots and Histograms.**

A wide variety of plotting tools are available including histograms and X-Y scatter plots, 2D,3D, 4D and 5D plotting available, print and export plots as images, selections made in a plot are directly linked to the chemical spreadsheet.

## **Perform Chemical and Mathematical Functions on a Chemical Spreadsheet or Local Database.**

A wide variety of functions are available for you to manipulate data contained within a chemical spreadsheet or database including calculating chemical properties on the fly, mathematical, arithmetical, transformation and unit conversion.

## **Apply QSAR Prediction Models**

Read in and apply QSAR prediction models built in ICM-Chemist-Pro.