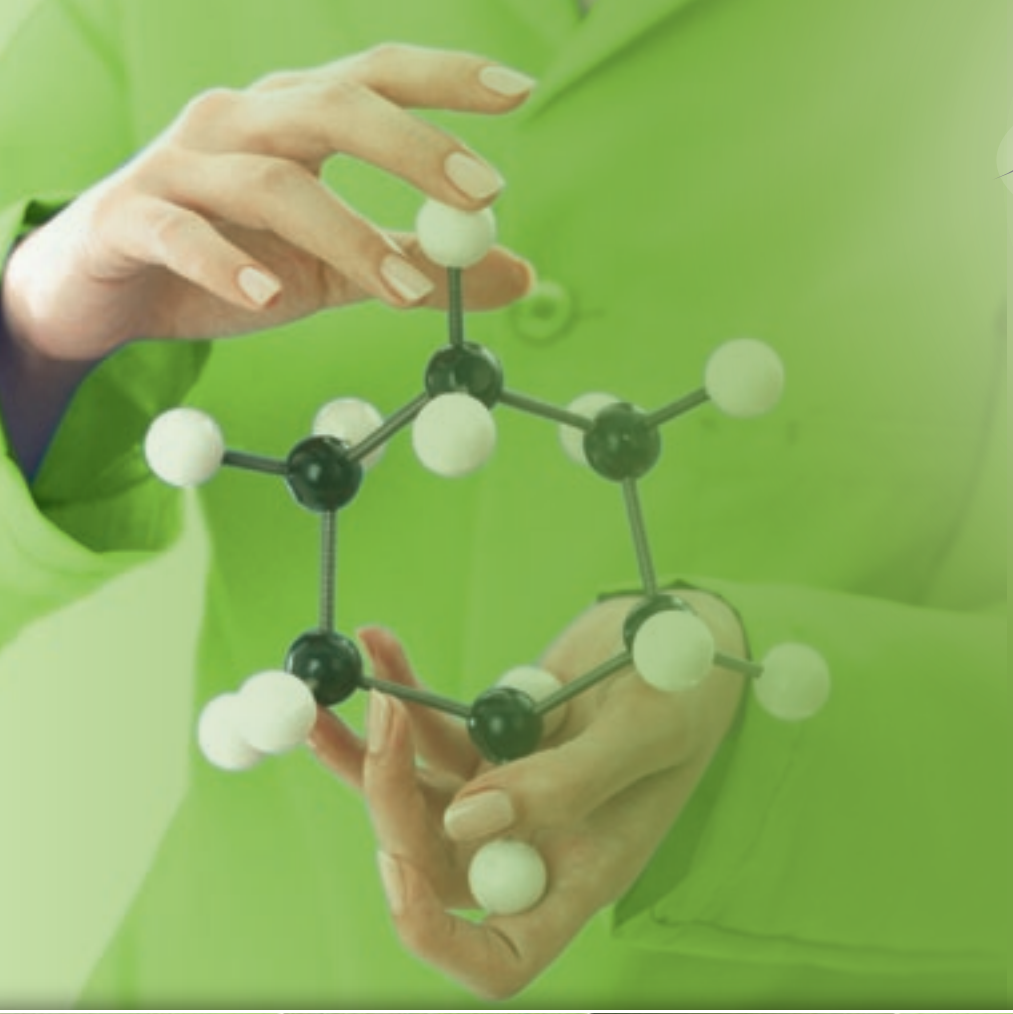
ChemXplor

Simplifying Computer Aided Discovery



Search multiple databases

Molecular fingerprints

Pharmacophoric features

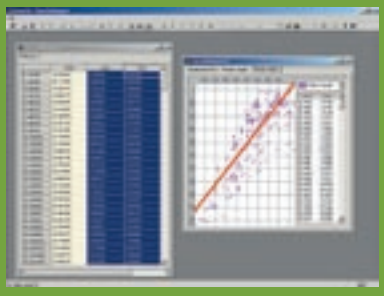
Substucture Search

Similarity & descriptor based searches

vLife Technologies

adding value to life

ChemXplor

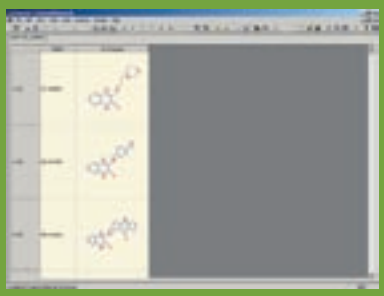


ChemXplor is comprehensive chemoinformatics software with extensive facilities for querying and building large-size compound databases. ChemXplor implements novel methodologies like Fingerprint based and pharmacophore based searches for advance applications. The software offers several combinations of quick and in-depth searches based on 2D / 3D substructures, similarity or descriptors. Researchers from industry and academia make use of ChemXplor for their database management and search requirements to arrive at better selection in lesser time using public as well as proprietary chemical databases.

ChemXplor also provides facilities for generating pharmacophoric features and subsequent database searches can be performed using these pharmacophoric features.

ChemXplor interfaces with other VLife products like VLifeMDS Engine, MolSign and LeadGrow. This enables users to seamlessly access supporting operations like molecule handling, conformation analysis, geometry optimization and combinatorial library generation

Salient Features



- Facilities to build and customize your own databases in line with your research requirements.
- Users can store every detail of the work including templates, queries (search conditions) and searched results from different databases to avoid repetition of any part of the work.
- Extensive facilities for automatic checks for molecular consistency during database creation itself to avoid disconnected or faulty molecular structures creeping into the database.
- Exhaustive search functions for rapid querying on multiple databases in one shot based on 2D substructures, 3D substructures, molecular similarities or molecular descriptors.
- Additional flexibility to fine-tune the searches by specifying a number of attributes (such as charge, hybridization, connectivity and so on to each atom of template) and suitable combinations of these attributes using many AND as well as OR conditions
- Molecular Fingerprint: The software provides facilities to create user-defined molecular fingerprints, customize & save the finger-print and query the compound databases using the saved fingerprint.
- User friendly result tables: The search results for different databases are displayed on different sections in the output window in result tables which support mathematical and table handling functions for ease of further sorting and other operations.
- Elevated searches: The software provides utilities for advanced searches like pharmacophore based searches and receptor based searches`

Technical features

- Completely designed by VLife's team of practicing scientists and technocrats
- Runs on **standard hardware** (Pentium 4 or AMD athlon or equivalent)
- Operates on **Windows Operating System**
- Easily customizable and simple for integration
- Object oriented framework and modular design

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