



JChem Base

Java based
structure
search engine
accessing
multiple
database types

JChem Base is the search and database bridge component of ChemAxon's Java based chemical software technology.

JChem Base enables database engines to search structural data and also serves to connect existing client database platforms, web servers, users and ChemAxon's growing suite of cheminformatics tools.

JChem Base can handle molecule, reaction, combinatorial Markush and query structural contents and associated data.

Searching

Structure based searching includes exact, substructure and similarity searches. Searches can combine structural and non structural data using JChem Base's search functions and SQL statements via JDBC.

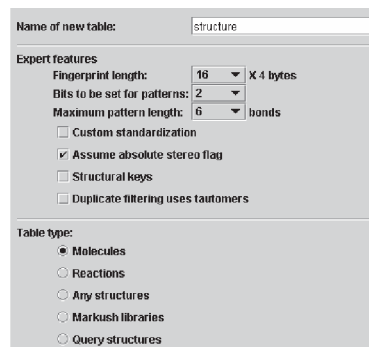
- Exact structure, substructure and superstructure matching
- Variable similarity searching including reaction similarity
- Generic query atoms and bonds, atom lists / not lists, pseudo atoms
- Supporting many query properties
- Full SMARTS support
- Reaction queries
- R-group query expressions
- Tautomer search
- Stereo specific structure and reaction specifications
- Structure canonicalization (integrated with Standardizer)

Administration

JChem Base comes with a GUI for database management, JChemManager, to create and drop tables or import and export structure files.



JChemManager interface



JChem Base Create Table dialogue

Oracle Cartridge

Using the JChem Cartridge for Oracle the user can access many chemical functions from within Oracle. SQL SELECT statements can combine structural searching, predictions, calculations etc.

Chemical Terms

ChemAxon's Chemical Terms is an extensible human understandable and machine processable language which allows users to formulate complex chemical questions, expressions and rules.

Chemical Terms can contain references to functional groups, other structural elements and physico-chemical properties. The language is used in two ways:

- Calculated columns are automatically filled during structure imports and updates, and can be used during search as any other column.
- Searches can include extra conditions formulated as Chemical Terms filters and evaluated on the fly.

Combinatorial Markush JChem Base add-on

Allows the registration of generic structures into the database and substructure and exact structure searching in their enumerated libraries (without enumeration of library members).

Currently handles the following generic features: R-groups (nested to any depth), atom and bond lists and link nodes.

Together with the Markush enumeration plugin simplifies the analysis of complex combinatorial Markush structures (libraries of complexity 10^{30} and above).

Integration

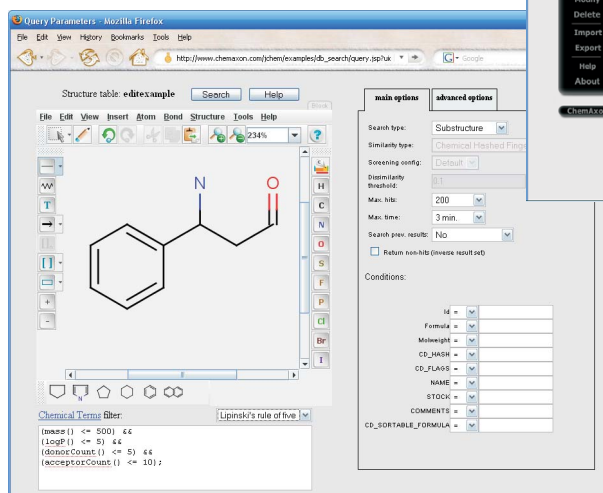
JChem Base is able to interact with many database types and can import and export many common chemistry file formats .

As a server side application based on Java technology and also accessible from .NET applications via JNBridge, JChem Base is built to fit into your existing IT network with a minimum of work and disturbance.

Instant JChem, our chemical database client tool can interact with JChem Base servers to share chemical and non-chemical data on the user desktop.

For inter/intra-net applications JChem Base supports JSP and ASP technology giving web managers a fast and rich interactive solution for delivering content.

- No chemical software needs to be present on the clients' system - requires only a browser and Java
- Includes Marvin structure drawing and viewing tools and core classes
- Compatibility with many database engines such as Oracle, MySQL, MS SQL Server, DB2, PostgreSQL, Access, etc
- MOL, MRV, RXN, SDF, RDF, SMILES files supported



- Highly customizable developer features
- Chemical and non chemical data can be handled
- BLOB support for Oracle interaction

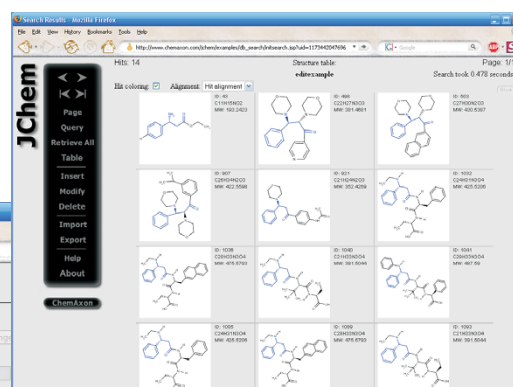
Support

For developers and users we have extensive support available.

- User and developer documentation, including API
- Searchable open access Technical Support Forum available
- Online feature demonstrations <http://www.chemaxon.com/jchem/examples.html>
- Response to all support requests on the same day, support issues usually resolved within days
- We welcome your feedback. It is used as the basis of our product development

About ChemAxon

ChemAxon is a leader in providing Java based chemical software development platforms for the biotechnology and pharmaceutical industries.



JChem Base JSP implementation, showing query structure, Lipinski's (rule of 5) Chemical Terms filter (left) and result with substructures aligned and color highlighted (above)

ChemAxon

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Online demo - www.chemaxon.com/jchem/examples/jsp1_x/index.jsp



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