JChem: Java Applets and Modules Supporting Chemical Database Handling from Web Browsers

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A Java based development tool for building portable chemical information systems is presented. The system contains applets for constructing web-based interfaces and classes that add structure handling to relational databases. Custom applications built with JChem can combine SQL and structural queries.

JChem is a tool for creating web applications that access chemical structures and corporate data in a database over the Internet or in Intranets. The front ends of such systems are HTML pages containing the Marvin Java Applets. The pages are generated by customized software pieces on the server, which use the JChem Class Library. Structures and other data are retrieved from a relational database management system (RDBMS).

PRINCIPLES APPLIED AT THE CREATION OF JCHEM

No Installation on the User's Machine. To keep the cost of setup and maintenance low, only a web browser has to be present on the user's machine to access a JChem application.

Portability. The software both on the user's machine and on the server run under practically every operating environment. Organizations applying JChem can tune the applications to their preferred operation system, web server, and database server, and moving to a new environment is smooth.

To achieve the above goals, all components of JChem were developed in Java.[1]

In a web application developed using JChem, users can enter or modify structures in a web browser using the MarvinSketch Java applet (Figure 1). For the display of molecules in a tabulated format, the MarvinView applet is provided. Both applets can export MDL Molfiles,[2] Sybyl Molfiles, and SMILES[3] (and a subset of SMARTS[4]) to the server or to an applet window, handle stereo bonds, and display automatically calculated charges and H atoms. For faster structure transfer, MDL Molfiles can be compressed to GZIP or to csmol[5] format. The latter one enables scripts on the server to insert compressed Molfiles into HTML files.

A few special features of MarvinSketch are valence checking, query atoms and bonds, and user-defined templates. Among other characteristics, MarvinView can magnify structures in a separate window, display textual information along with molecules, and rotate structures in 3D. Special controls (check boxes and buttons) can be inserted into a structure table. The basic functionality of the applets is stored in the marvin.jar file that is downloaded automatically at the first usage. Despite the several features included in the applets, the size of marvin.jar is only 78K in version 2, due to the modularity applied, which allows downloading only those modules that are actually needed. Swing[6] capable browsers can use the friendlier Swing version of the applets.

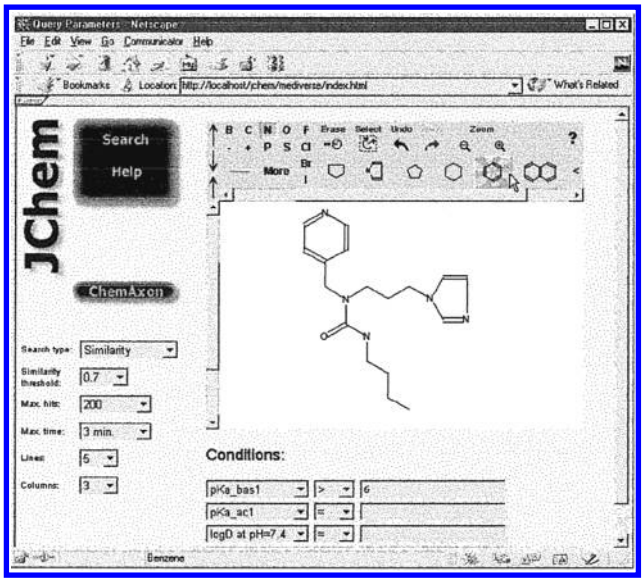

Figure 1. HTML page containing MarvinSketch.

JChem can store structures in almost any of the current relational database systems, from commercial database servers, such as Oracle, to free ones, such as MySQL. The only requirement is that the system must be supplied with an appropriate (JDBC[7]) driver for the database to access data from Java. Structure tables can be generated and structures can be imported and exported using JChemManager, a Java application available in both a command line and graphical interface mode.

To generate HTML pages accessing structures in a database, servlets[8] or Java Server Pages (JSP)[9] can be built, which call JChem objects (Figure 2). JChem provides substructure and similarity searching and molecule update and retrieval for these modules. Since Java is a general-purpose language, the modules can also perform other complex tasks. Combining structural and nonstructural (even nonchemical) data in the database allows connecting structure searches with regular SQL queries, which is advantageous compared to traditional structure handling software. Of

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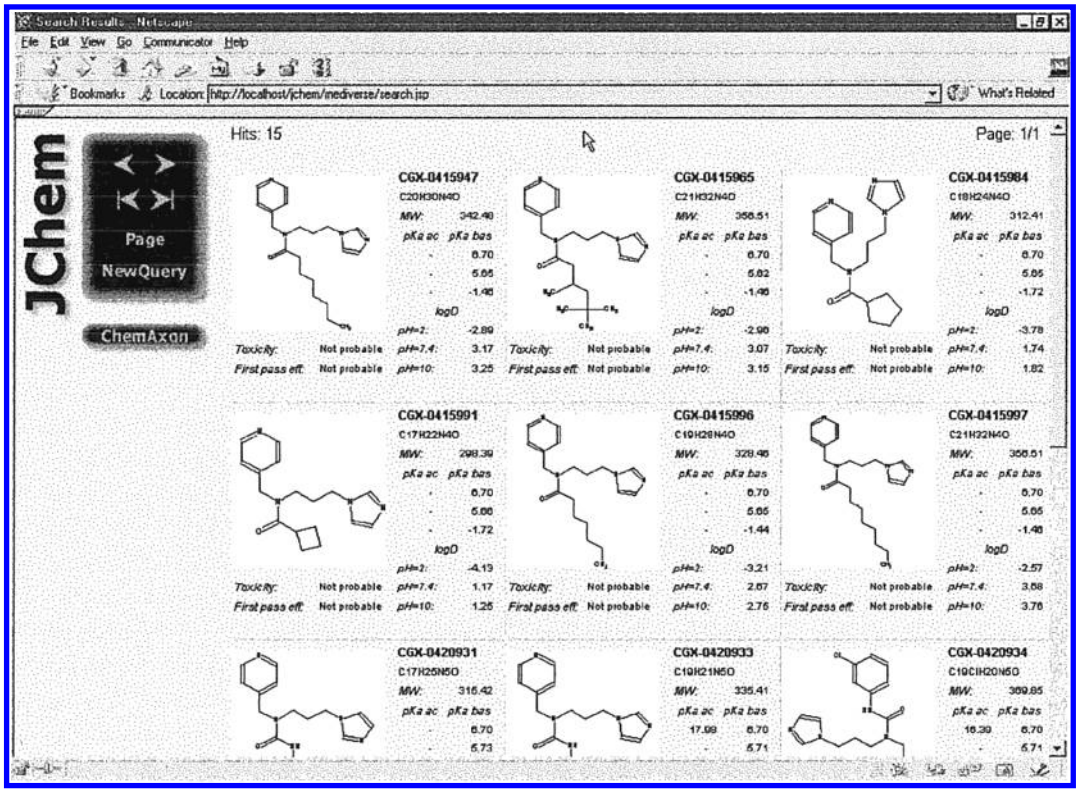

Figure 2. Search results in a MarvinView table generated using JChem.

course, it is also possible to combine servlets with CGI or other types of server side scripting, which enables building structure handling into legacy systems.

SYSTEM REQUIREMENTS

Marvin Applets. Any Java capable web browser.

Server Side Modules Using JChem Class Library. Java Runtime Environment 1.1 or above, any web server running servlets, and any database server that is supplied with a JDBC or ODBC driver.

JChemManager. Java Runtime Environment 1.1 with the Swing class library, or Java Runtime Environment 1.2 or above

All operating systems that run the above software are applicable to run JChem's components. The software is available from ChemAxon (http://www.chemaxon.com). Marvin Java Applets are free for publicly available Internet sites.

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