Interfacing the JChem Suite outside of Java

Jonathan Lee

ChemAxon

Solutions for Cheminformatics

Outline

- JChem Interfaces
- Situational Factors
- SQL
- .NET
- Web Services
  - Details
  - Demo
- Workflow Integrations

Interfaces to JChem Suite of Tools

Java

- Direct POJO and Server-side JSP

SQL

- JChem Cartridge for environments with Oracle

.NET

- Interoperability with .NET framework

Web Services

- Platform and Language-Independent

Situational Factors

Applicable Language

- Does Java, .NET, SQL, or other Web language figure prominently?

Data Environment

- Is Oracle the target structure database?

End User Environment

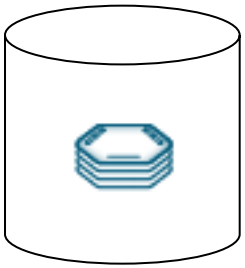
- Will the user have a Desktop Client or a Web Client?

Overall Technical Architecture

- Do you use a Service Oriented Architecture?

JChem Cartridge

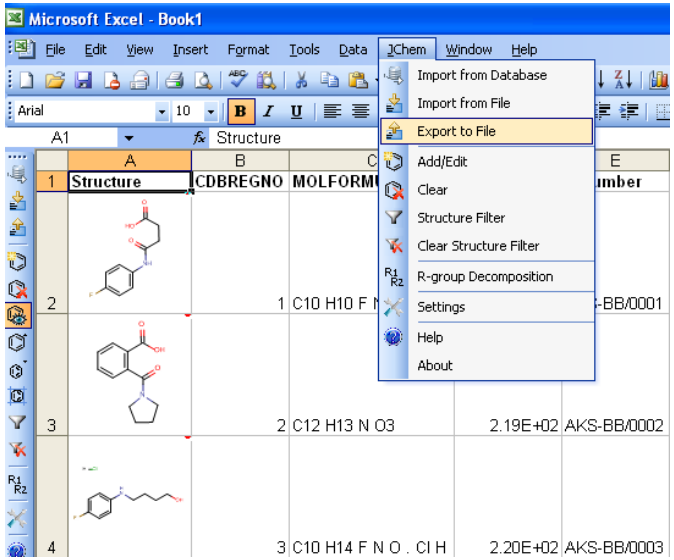
- Leverage Oracle Database Advantages
- Stored procedures quickly handle database work
- External communication with JChem Server for process intensive work



Supports
•SQL
•Most JChem Modules (Searching, Standardization, Reactor, Chemical Terms, Calculator Plug-in, …)

.NET

- Pure .NET solution for all non-GUI elements
- Marvin .NET GUI components (Marvin 5.3)
- New no cost native .dll is simpler, faster, than earlier JNBridge solution



Supports

•All .NET languages (C#, VB.NET, …)

•All of JChem Suite (except Cartridge and Marvin Beans classes)

JChem Web Services

- WS-I, SOAP, and WSDL standards
- Reusable and accessible to other services
- Automated client-side code generation

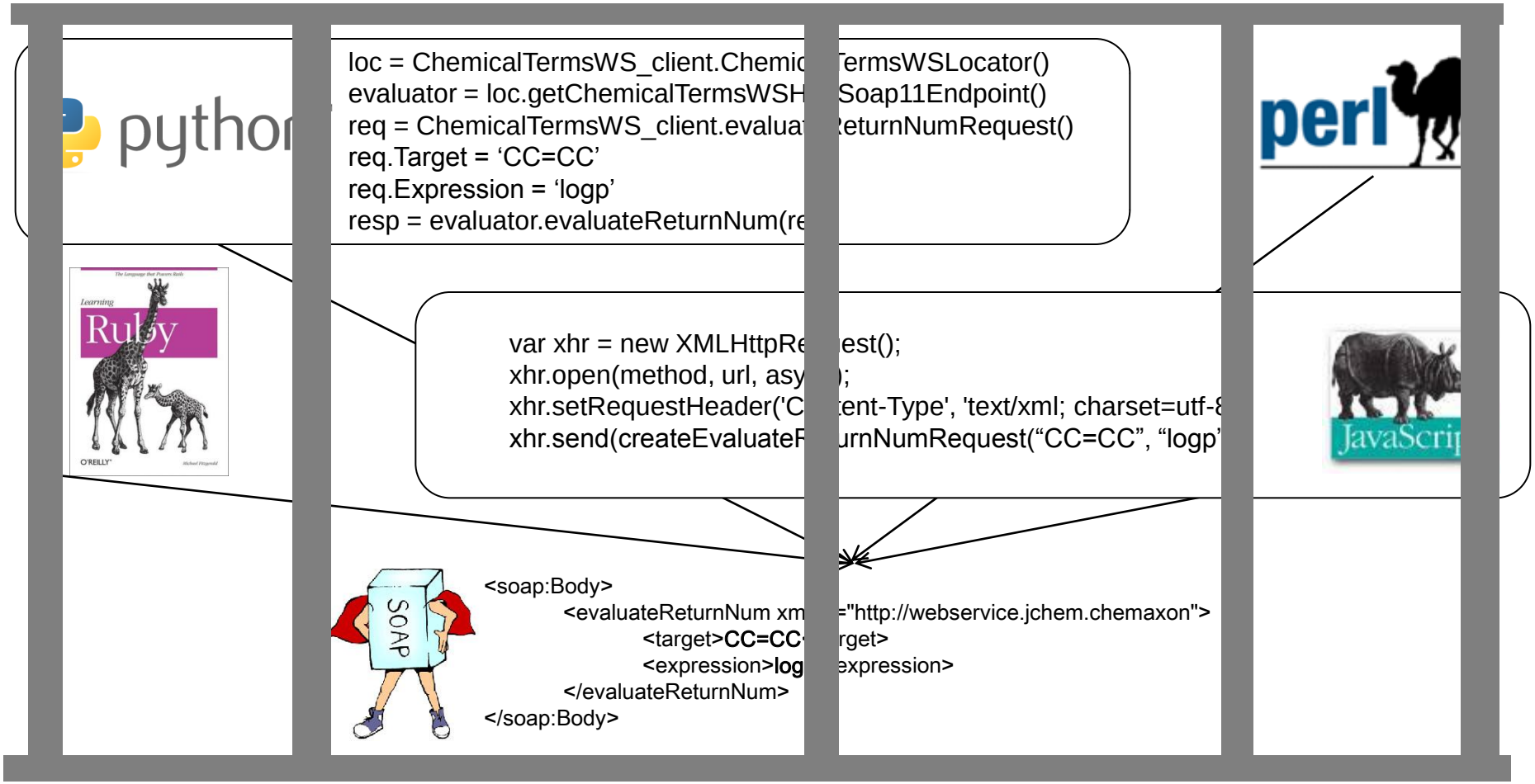
Supports

•Web Languages: AJAX/JavaScript, Perl, Python, Ruby, PHP, …

•App languages: Java, C#, …

•Growing list of JChem Modules (Searching, Standardization, Chemical Terms, Molecule Conversion)

Unlocking the Scripting Menagerie

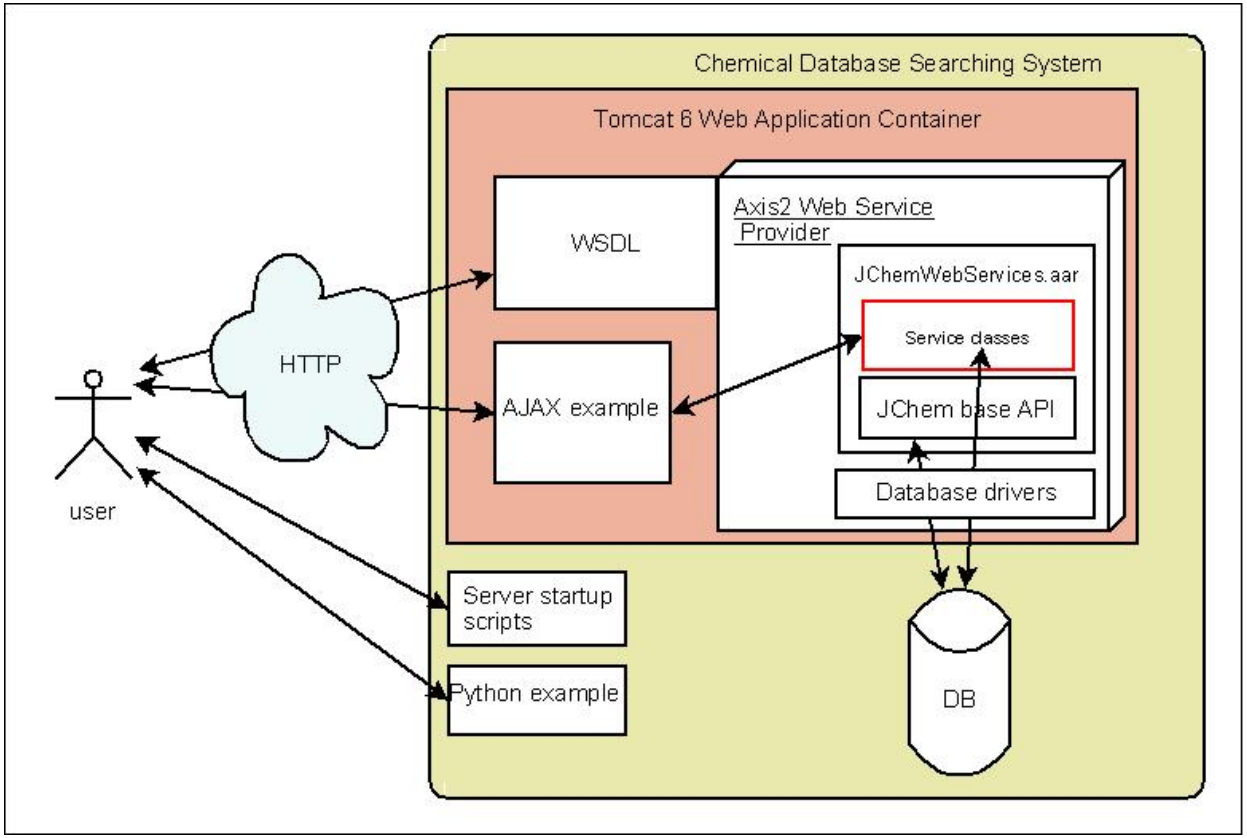


JChem Web Services

JChem WS Server Architecture

Apache Open Source Components

- Axis2 Web Service Engine and Tomcat Web Container



OS List

- Windows
- Unix
- Linux (SUSE, Red Hat, Ubuntu, Gentoo)
- Mac OS X

Current and Future Services

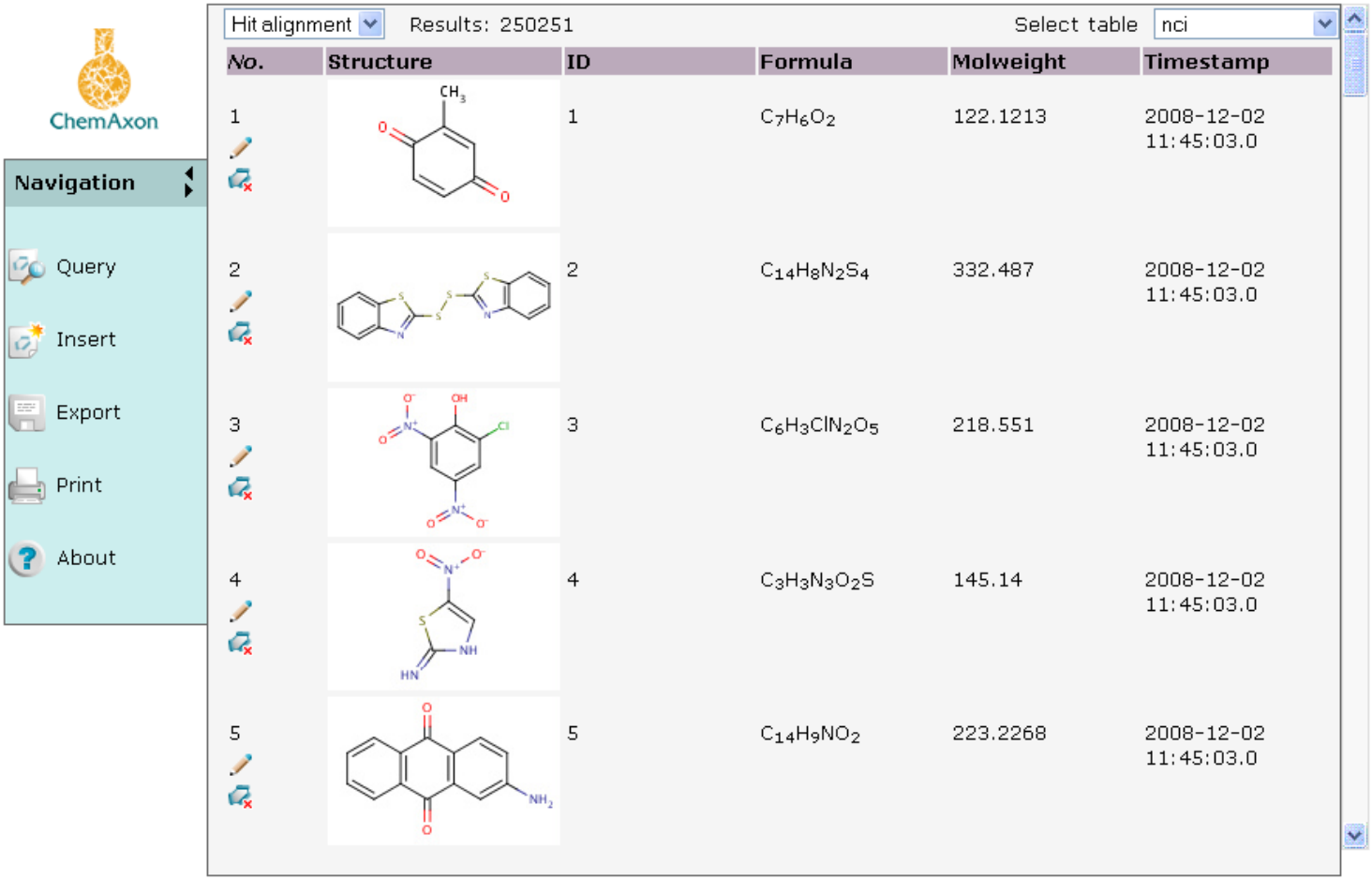
- JChem Search Service
- Standardization Service
- Molecular Conversion Service
- Chemical Terms Evaluation Service

Future Enhancements

- Reactor
- SQL Execution
- Relational Table Searching
- Data Manipulation
- Batch Processing

AJAX Demo of JChem Web Services

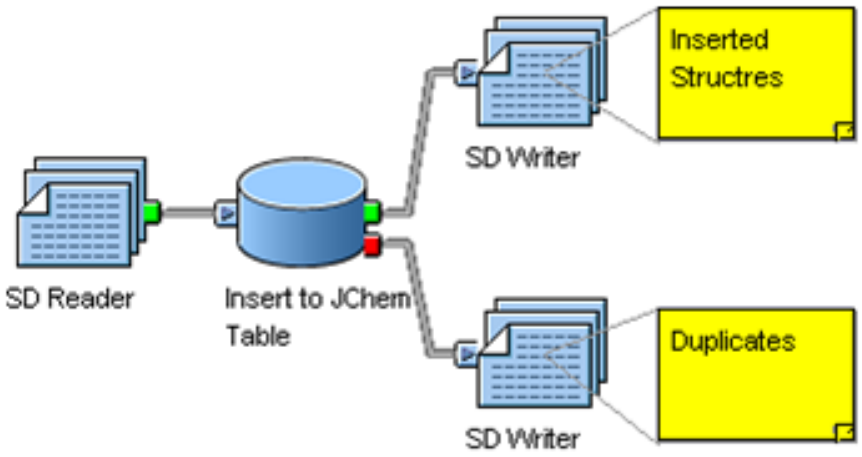
JChemSearch Web Service - www.chemaxon.com/ajax



Workflow Integrations

ChemAxon components exist for several workflow software vendors

- Accelrys Pipeline Pilot
- KNIME Workbench (by Infocom)
- Inforsense Analytics



Find out more about JChem Cartridge

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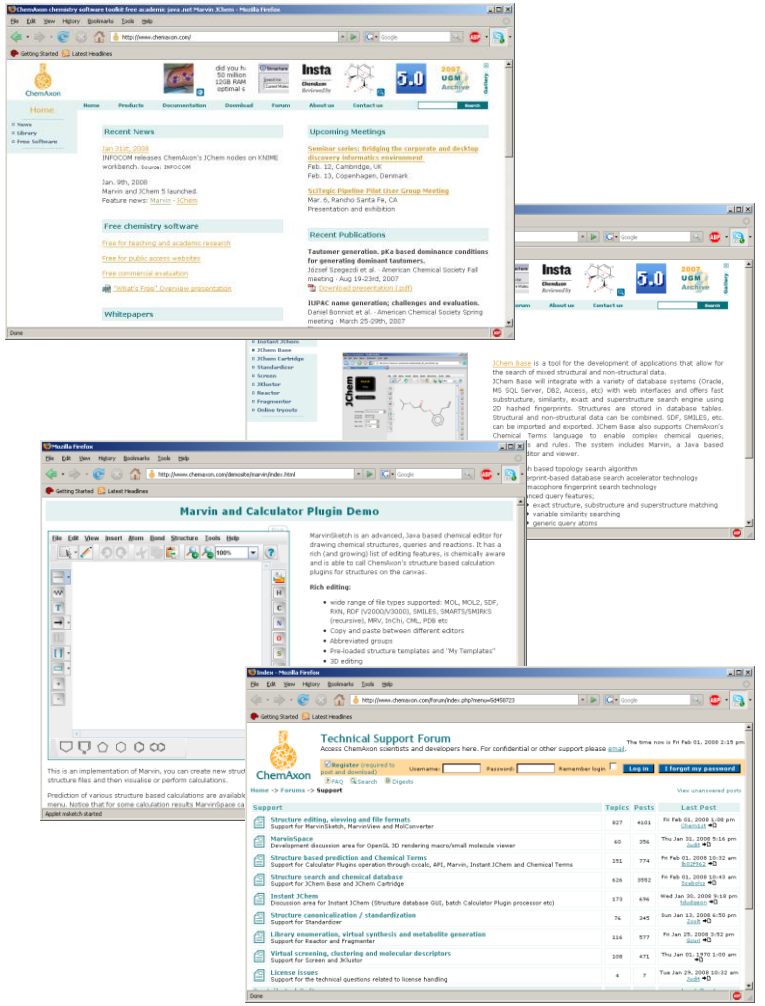

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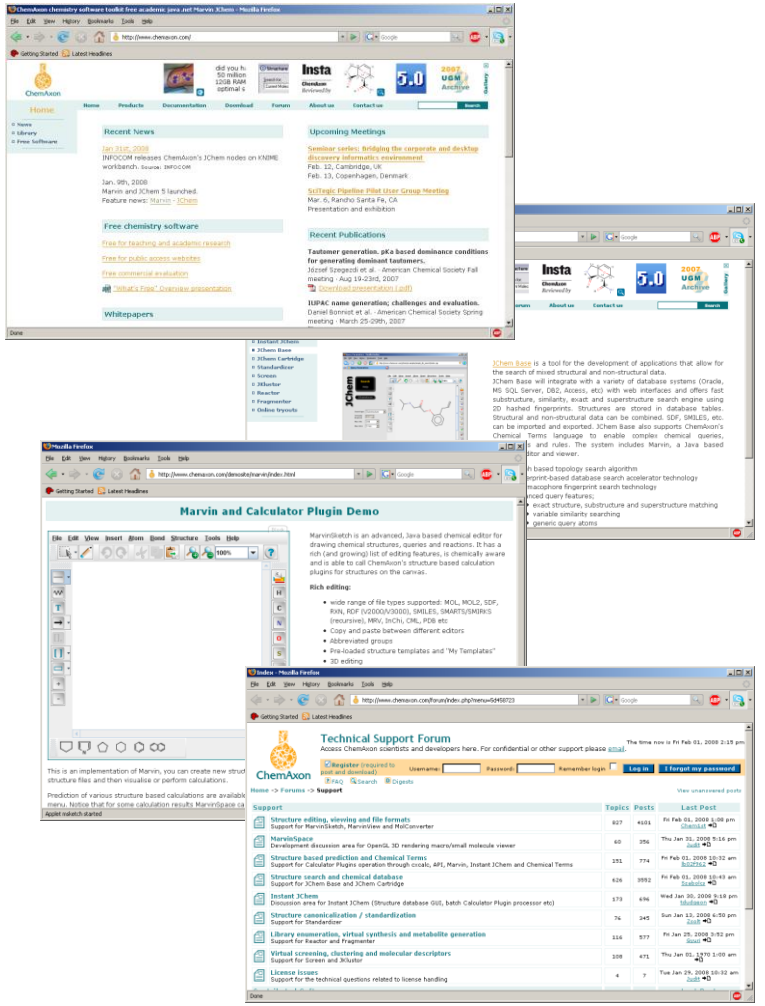

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