

# Interfacing the JChem Suite outside of Java

**Jonathan Lee**

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

# Interfaces to JChem Suite of Tools

**Visualization**

**Marvin**  
Structure, query & reaction editor, viewer & visualization

**Property prediction**

**Calculator Plugins**  
Structure property prediction & calculation

**Selected calculations listing**

- pKa, Major microspecies
- logP, logD
- Charge
- Tautomerization
- Stereoisomer
- Conformation and 3D alignment
- Topology Analysis
- Molecular Surface Area
- Markush Enumeration
- Hydrogen Bond Donor-Acceptor
- Structural Frameworks
- Structure to Name
- ...etc.

**Add-on's**

**Chemical DB - toolkit**

**JChem Cartridge**  
JChem/Oracle integration

**JChem Base**  
Structure searching & db access

**Standardizer**  
Chemical canonicalization / business rules

**Chemical DB - desktop**

**Instant JChem**  
Structure db management, search & prediction

**JChem for Excel®**  
Enabling chemistry in Excel

**Visualization**

**Name to Structure**  
Converting chemical names to structures

**Enumeration**

**Reactor**  
Enumeration via reaction modelling

**Metabolizer**  
Metabolic pathway & stability prediction

**Library analysis**

**JKluster**  
Clustering & diversity analysis

**Fragmenter**  
Decomposition to fragments and R-groups

**Screen**  
HT pharmacophore screening



## 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

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## 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?

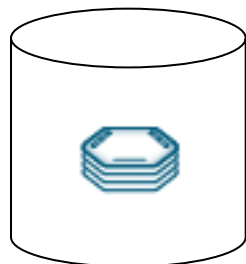
## Overall Technical Architecture

- 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

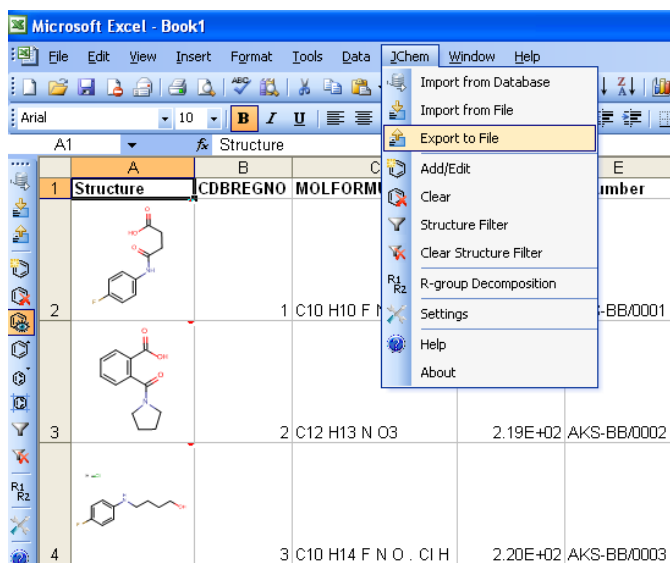
**ORACLE®**



## Supports

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

- 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

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



## Supports

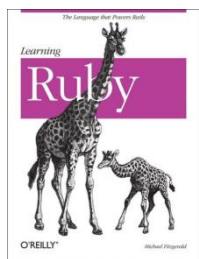
- Web Languages: AJAX/JavaScript, Perl, Python, Ruby, PHP, ...
- App languages: Java, C#, ...
- Growing list of JChem Modules (Searching, Standardization, Chemical Terms, Molecule Conversion)

# Unlocking the Scripting Menagerie

python

```
loc = ChemicalTermsWS_client.ChemicalTermsWSLocator()
evaluator = loc.getChemicalTermsWSHTTP(Soap11Endpoint())
req = ChemicalTermsWS_client.evaluator.evaluateReturnNumRequest()
req.Target = 'CC=CC'
req.Expression = 'logp'
resp = evaluator.evaluateReturnNum(req)
```

perl 



```
var xhr = new XMLHttpRequest();
xhr.open(method, url, async);
xhr.setRequestHeader('Content-Type', 'text/xml; charset=utf-8');
xhr.send(createEvaluateReturnNumRequest("CC=CC", "logp"))
```



```
<soap:Body>
  <evaluateReturnNum xmlns="http://webservice.jchem.chemaxon">
    <target>CC=CC</target>
    <expression>logp</expression>
  </evaluateReturnNum>
</soap:Body>
```

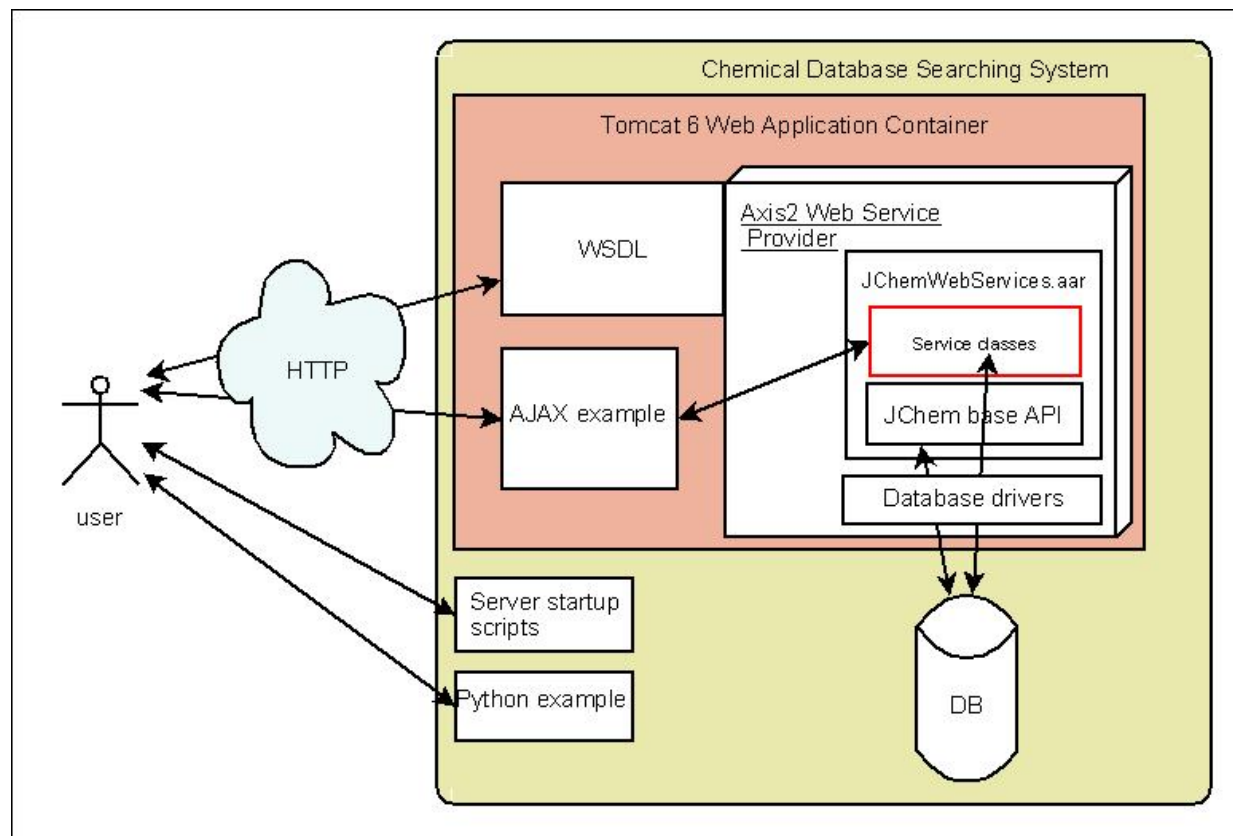


JChem Web Services

# 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

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- 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

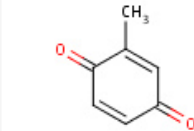
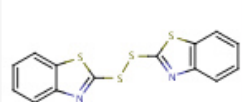
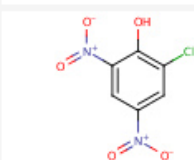
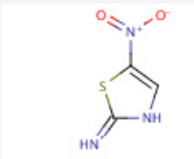
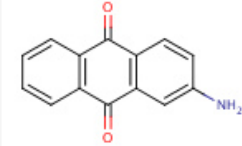
JChemSearch Web Service - [www.chemaxon.com/ajax](http://www.chemaxon.com/ajax)

  
ChemAxon

**Navigation**

- Query
- Insert
- Export
- Print
- About

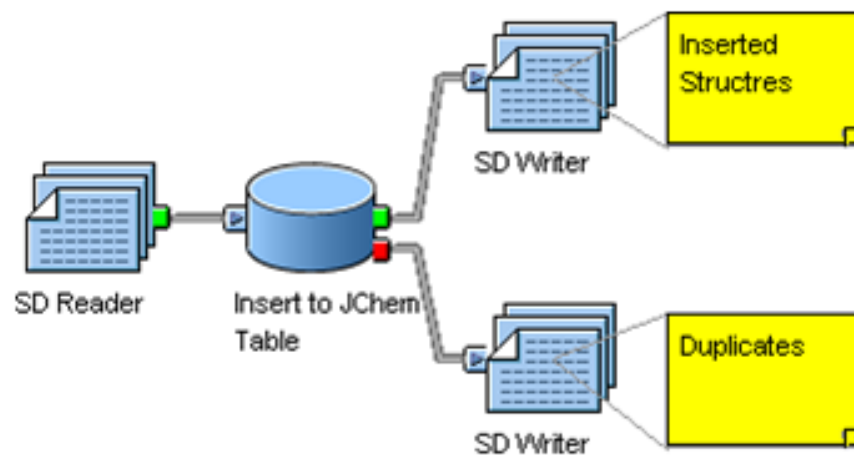
Hit alignment  Results: 250251 Select table

No.	Structure	ID	Formula	Molweight	Timestamp
1		1	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	122.1213	2008-12-02 11:45:03.0
2		2	C <sub>14</sub> H <sub>8</sub> N <sub>2</sub> S <sub>4</sub>	332.487	2008-12-02 11:45:03.0
3		3	C <sub>6</sub> H <sub>3</sub> ClN <sub>2</sub> O <sub>5</sub>	218.551	2008-12-02 11:45:03.0
4		4	C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S	145.14	2008-12-02 11:45:03.0
5		5	C <sub>14</sub> H <sub>9</sub> NO <sub>2</sub>	223.2268	2008-12-02 11:45:03.0

# 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

- **Product descriptions & links**

[www.chemaxon.com/product/jc\\_cartridge.html](http://www.chemaxon.com/product/jc_cartridge.html)

- **Forum**

[www.chemaxon.com/forum/forum7.html](http://www.chemaxon.com/forum/forum7.html)

- **Presentations and posters**

[www.chemaxon.com/conf/JChemCartridge.ppt](http://www.chemaxon.com/conf/JChemCartridge.ppt)

- **Download**

[www.chemaxon.com/jchem/download.html](http://www.chemaxon.com/jchem/download.html)

The collage includes several screenshots:

- ChemAxon Website Home:** Shows the 'Recent News' section with headlines such as 'INFOCAMP releases ChemAxon's JChem nodes on KNDNE workbench', 'Free chemistry software', and 'Customer generation, pKa based dominance conditions for generating dominant tautomers'.
- Harvin and Calculator Plugin Demo:** A screenshot of the Harvin software interface showing a chemical structure editor with various toolbars and a rich editing menu.
- Technical Support Forum:** A screenshot of the forum page with a search bar and a table of support topics and posts.

Support	Topics	Posts	Last Post
Structure editing, viewing and file formats	827	4081	Feb 01, 2008 1:00 pm
Support for MarvinSketch, MarvinView and MarvinCenter			Deleted
MarvinSpace	60	306	Feb 01, 2008 11:16 pm
Environment discussion area for OpenBabel, 3D rendering, macros/email molecule viewer			Deleted
Structure based prediction and Chemical Terms	351	174	Feb 01, 2008 10:02 am
Support for Calculator Plugins operation through Oracle, API, Marvin, Instant JChem and Chemical Terms			Deleted
Structure search and chemical database	426	1982	Feb 01, 2008 10:43 am
Support for JChem Base and JChem Cartridge			Deleted
Instant JChem			Deleted
Discussion area for Instant JChem (Structure database GUI, both Calculator Plugin processor etc)	173	416	Wed Jan 30, 2008 9:10 pm
Structure conversion/alignment / standardization	76	345	Wed Jan 30, 2008 11:30 pm
Library enumeration, virtual synthesis and metabolite generation	116	517	Feb 01, 2008 1:02 pm
Support for Reactor and Fragmenter			Deleted
Virtual screening, clustering and molecular descriptors	308	471	Feb 01, 2008 1:00 pm
Support for Solver and Shaper			Deleted
License Issues	4	1	Feb 01, 2008 10:12 am
Support for the technical questions related to license handling			Deleted

# Find out more about .NET integration

- **Product descriptions & links**

[www.chemaxon.com/NET\\_support\\_land.html](http://www.chemaxon.com/NET_support_land.html)

- **Forum**

[www.chemaxon.com/forum/forum7.html](http://www.chemaxon.com/forum/forum7.html)

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The collage includes several screenshots:

- ChemAxon Homepage:** Features sections for 'Recent News' (e.g., 'INFOCOM releases ChemAxon's JChem nodes on KXNDE'), 'Upcoming Meetings' (e.g., 'Seminars series: Bridging the corporate and desktop'), and 'Recent Publications' (e.g., 'Customer generation, pKa based dominance conditions').
- JChem Base:** A screenshot of the software interface with a text box stating: 'JChem Base is a tool for the development of applications that allow for the search of mixed structural and non-structural data. JChem Base will integrate with a variety of database systems (Oracle, MS SQL Server, DB2, Access, etc) with web interfaces and offers fast substructure, similarity, exact and superstructure search engines using 2D hashed fingerprints. Structures are stored in database tables. Structural and non-structural data can be combined. DSF, SMILES, etc. can be imported and exported. JChem Base also supports ChemAxon's Chemical Terms language to enable complex chemical queries and rules. The system includes Marvin, a Java based editor and viewer.'
- Marvin and Calculator Plugin Demo:** A screenshot of the Marvin editor interface with a text box stating: 'Marvin is an advanced, Java based chemical editor for drawing chemical structures, queries and reactions. It has a rich (and growing) list of editing features, is chemically aware and is able to call ChemAxon's structure based calculation plugins for structure on the canvas.' It lists features like 'Rich editing' and 'Wide range of file types supported'.
- Technical Support Forum:** A screenshot of the forum interface with a search bar and a table of support topics.

Support	Topics	Posts	Last Post
Structure editing, viewing and file formats	827	4081	Fri Feb 05, 2009 1:00 pm
Support for MarvinSketch, MarvinView and PdfConverter	40	306	Thu Jan 31, 2009 5:16 pm
MarvinSpace	60	306	Thu Jan 31, 2009 5:16 pm
Development discussion area for OpenBabel, 3D rendering macros/email molecule viewer	351	374	Fri Feb 03, 2009 10:02 am
Structure based prediction and Chemical Terms	426	1092	Fri Feb 03, 2009 10:43 am
Support for Calculator Plugins operation through Oracle, API, Marvin, Instant JChem and Chemical Terms	179	496	Wed Jan 29, 2009 9:10 pm
Structure search and chemical database	76	245	Wed Jan 29, 2009 9:10 pm
Support for JChem Base and JChem Cartridge	116	577	Fri Jan 23, 2009 3:52 pm
Instant JChem	308	471	Thu Jan 22, 2009 10:00 am
Discussion area for Instant JChem (Structure database GUI, both Calculator Plugin processor etc)	4	7	Thu Jan 22, 2009 10:02 am
Structure conversion algorithm / standardization			
Support for MarvinView			
Library enumeration, virtual synthesis and metabolite generation			
Support for Reactor and Fragmenter			
Virtual screening, clustering and molecular descriptors			
Support for Solver and Shaper			
License Issues			
Support for the technical questions related to license handling			

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**Recent News**

- INFOCOM releases ChemAxon's JChem nodes on KXNIE workbench, source: zeroc.com
- Jan 26, 2008
- Marvin and Chem 5 launched
- Feature news: [Marvin](#) - [Chem](#)

**Free chemistry software**

- [Free for teaching and academic research](#)
- [Free for public access websites](#)
- [Free commercial evaluation](#)
- ["MolVec's Trick" - Chemistry generation](#)

**Whitepapers**

**Upcoming Meetings**

- Seminar series: Bridging the corporate and desktop business informatics environment**  
Feb. 12, Cambridge, UK  
Feb. 13, Copenhagen, Denmark
- Software Pipeline Pilot User Group Meeting**  
Mar. 6, Rancho Santa Fe, CA  
Presentation and exhibition

**Recent Publications**

- Topology generation, pKa based dominance conditions for generating dominant tautomers.**  
Norval Spradell et al. - American Chemical Society Fall meeting - Aug 19-23rd, 2007  
[View publication statistics](#)
- IUPAC name generation, challenges and evaluation.**  
Daniel Borrmann et al. - American Chemical Society Spring meeting - March 25-29th, 2007

**JChem Base** is a tool for the development of applications that allow for the search of mixed structural and non-structural data. JChem Base will integrate with a variety of database systems (Oracle, MS SQL Server, DB2, Access, etc.) with web interfaces and offers fast substructure, similarity, exact and superstructure search engine using 2D hashed fingerprints. Structures are stored in database tables. Structural and non-structural data can be combined. IUPAC SMILES, etc. can be imported and exported. JChem Base also supports ChemAxon's Chemical Terms language to enable complex chemical queries and rules. The system includes Marvin, a Java based editor and viewer.

**Marvin and Calculator Plugin Demo**

Marvinbatch is an advanced, Java based chemical editor for drawing chemical structures, queries and reactions. It has a rich (and growing) list of editing features, is chemically aware and is able to call ChemAxon's structure based calculation plugins for structures on the canvas.

**Rich editing:**

- wide range of file types supported: MOL, MOL2, SDF, RXN, RCF (V2000/V3000), SMILES, SMARTS/SMARTS (Impure), MW, ICHN, CML, PDB etc.
- Copy and paste between different editors
- Addressed groups
- Pre-loaded structure templates and "My Templates"
- 3D editing

**Technical Support Forum**

Access ChemAxon scientists and developers here. For confidential or other support please email [support@chemaxon.com](mailto:support@chemaxon.com)

Support	Topics	Posts	Last Post
Structure editing, viewing and file formats Support for MarvinBatch, MarvinViewer and FileConverter	827	4181	Fri Feb 01, 2008 9:00 am Detailed...
MarvinSpace Development discussion area for Open3D, 3D rendering, main/molecule viewer	60	306	Thu Jan 31, 2008 9:16 pm Detailed...
Structure based prediction and Chemical Terms Support for Calculator Plugin operation through Oracle, MS SQL, Marvin, Instant JChem and Chemical Terms	351	374	Fri Feb 01, 2008 10:02 am Detailed...
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Structure conversion/translation / standardization Support for Standardizer	76	345	Wed Jan 30, 2008 9:30 pm Detailed...
Library enumeration, virtual synthesis and metabolite generation Support for Reactor and Fragmenter	116	577	Fri Jan 25, 2008 9:52 am Detailed...
Virtual screening, clustering and molecular descriptors Support for Screen and Shaper	308	471	Thu Jan 24, 2008 1:00 am Detailed...
License Issues Support for the technical questions related to license handling	4	7	Tue Jan 29, 2008 10:32 am Detailed...